Boosting the Photovoltaic Performance of an Inverted P3HT:PCBM Based Bulk hetero-junction Organic Solar Cell

Murad Jemal Husen

A Thesis Submitted to the department of Applied Physics

School of Applied Natural Science

Presented in Partial Fulfillment of the Requirement for the Master's Degree in Applied physics (Material Physics)

Office of Graduate Studies

Adama Science and Technology University

June, 2022

Adama, Ethiopia

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Advisor: Solomon Tiruneh Dibaba (PhD)

Co-advisor: Fekadu Gochole Aga (PhD)

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Declaration

I hereby declare that this Master Thesis entitled “Boosting the Photovoltaic Performance of an Inverted P3HT: PCBM Based Bulk hetero-junction Organic Solar Cell” is my original work. That is, it has not been submitted for the award of any academic degree, diploma or certificate in any other university. All sources of materials that are used for this thesis have been duly acknowledged through citation.

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Recommendation

We, the advisors of this thesis, hereby certify that we have read the revised version of the thesis entitled “Boosting the Photovoltaic Performance of an Inverted P3HT: PCBM Based Bulk hetero-junction Organic Solar Cell” prepared under our guidance by Murad Jemal submitted in partial fulfillment of the requirements for the degree of Mater’s of Science in material physics. Therefore, we recommend the submission of revised version of the thesis to the department following the applicable procedures.

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Co-advisor	Signature	Date

Approval Page

We, the advisors of the thesis entitled "Boosting the Photovoltaic Performance of an Inverted P3HT: PCBM Based Bulk hetero-junction Organic Solar Cell" hereby certify that the recommendation and suggestions made by the board of examiners are appropriately incorporated into the final version of the thesis.

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Co-advisor	Signature	Date

We, the undersigned, members of the Board of Examiners of the thesis by Murad Jemal have read and evaluated the thesis entitled "Boosting the Photovoltaic Performance of an Inverted P3HT: PCBM Based Bulk hetero-junction Organic Solar Cell" and examined the candidate during open defense. This is, therefore, to certify that the thesis is accepted for partial fulfillment of the requirement of the degree of Master of Science in material physics.

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Acronyms

Ag…….Silver

BHJ……..……Bulkhetrojunction

CdTe……Cadmium Telluride

CIGS……....Copper Indium Gallium Selenide

EMR…….…...Electromagnetic Radiation

ETL……..Electron Transport Layer

FF…….Fill Factor

GPVDM……..General Purpose Photovoltaic Device Model

HOMO…….Highest Occupied Molecular Orbital

HTL…….....Hole Transport Layer

ITO…….....Indium Tin Oxide

J_{max}.....Maximum Current

J_{sc}……..……Short Circuit Current Density

LUMO…….…….Lowest Unoccupied Molecular Orbital's

MoO_3…….….Molybdenum Trioxide

OPV…….Organic Photovoltaic

OSC……..Organic Solar Cell

PCBM……..Phenyl-C61-butyric acid methyl

P3HT…….. ..Poly (3-hexylthiophene)

R_{pm}……Revolution per minute

V_{max}…….……Maximum Voltage

V_{oc}……Open Circuit Voltage

Abstract

In this thesis, the effect of active layer thickness, hole transport layer thickness and electron mobility for P3HT: PCBM based inverted organic solar cell has been investigated. Numerical simulation for the structure ITO/ZnO /P3HT: PCBM/MoO_3/Ag has been done using General Purpose Photovoltaic Device Model (GPVDM) program tool. The short circuit current density (Jsc), open circuit voltage (Voc), fill factor (FF) and power conversion efficiency (PCE) of the cell demonstrated by varying the thickness of active layer from 140 nm to 240 nm ,hole transparent layer from 1 nm to 60 nm and electron mobility from 50 $nm^2v^{-1}S^{-1}$ to 650 nm^2 $V^{-1}S^{-1}$. The performance improvement was observed at 220 nm and 20 nm active layer and hole transporting layer thickness respectively at $4.5x10^{-7}m^2V^{-1}S^{-1}$ *electron mobility. The demonstration result shows the thickness of active layer, hole transport layer and charge carrier mobility plays important role for performance improvement of organic solar cells.*

Keywords GPVDM software, P3HT: PCBM, Bulk-heterojunction solar cell, active layer, power conversion efficiency

CHAPTER ONE

INTRODUCTION

1.1 Background

The energy demand has increased significantly due to the high consumption of electricity, elevation in the world population, and industrial dependency on electricity rather than fossil fuels. Technological advances in electronics and automotive industries require a high input of energy. Considering the high demand for energy consumption, lack of conventional energy supplies, and their adverse effects on the environment, it is becoming crucial to start making use of unconventional energy resources, renewable energy and to restructure the traditional processes to increase energy efficiency(Lakatos et al., 2011).

However, to fully realize the utilization of green and renewable energy sources, such as solar energy, wind, and biomass, there is a critical need for energy storage. The application of solar energy in addressing global energy and environmental issues has recently attracted increasing attention and various techniques for the same have emerged. Solar energy can be converted directly into electrical or chemical energy through photovoltaic or photo electrochemical cells and photo catalysis, respectively (Aga et al., 2022), which is generally governed by five processes: (i) Photon absorption,(ii) Exciton diffusion,(iii) Exciton dissociation,(iv) Free carrier transport, and (v) Free carrier collection (Tran et al., 2020).

Photovoltaic devices that convert solar energy into electrical power are mainly divided into two types; organic and inorganic. Inorganic based solar cells have enhanced substantially over the last three decades. As a major breakthrough, the first inorganic solar cell (silicon based) was developed in 1954 by Bell labs. Since then, the power conversion efficiency for silicon solar cells has been improved from 6% to 31%. However, there are major limitations with these solar cells including the environmental toxicity, high cost of materials, complex fabrication processes, high capital cost for commercialization, and heavy weight of the operating solar. Organic solar cells, on the other hand, have many advantages over inorganic solar cells. It is charging low prices to produce the materials and easy fabrication processes. They are also robust, flexible, and lightweight(Kana, 2011). Organic solar cells mainly consist of small organic molecules or conducting polymers as a donor and accepter. Furthermore, these materials are easily fine-tuned through synthetic modifications to match the full absorption region of the solar spectrum.

The optical absorption coefficient of organic molecules is high so a large amount of light can be absorbed with a small amount of materials. In last two decay Organic based solar cell technologies have been a very attractive area of research. Bulk hetero-junction (BHJ) organic solar cell is being widely investigated in recent days. In BHJ photon absorption and generation of excitons(hole-electron pair) occurs at the donor-acceptor blend. Hole electron pair are splitted at donor-acceptor interface and separated charges are transported to opposite electrodes though active material. Among various donor - acceptor combinations, P3HT as donor and PCBM as acceptor have been seen to be quite efficient due to its high crystalline, large absorption in red region, and high hole mobility degree. Between the electrodes and active layer, MoO_3 and ZnO is used as buffer layers to block the electron and hole transfer in wrong direction(Sen & Bengal, 2019).

In OSC, conjugated organic polymers are used to absorb the incident light and for transporting the charge in order to produce electricity. Organic solar cell cover larger range of surfaces than inorganic solar cells and the manufacturing costs are significantly lower than the conventional inorganic solar cells. They also can be processed easily than inorganic solar cells(Sahare, 2016). It is called BHJ solar cells as electron donor and acceptor materials are blended in a disordered orientation which limits its PCE. In order to improve the power conversion efficiency and performance, we have changed the layer thickness and electron mobility to observed the characteristics curve which we have generated using General-Purpose Photovoltaic Device Model (GPVDM). It is a free general-purpose software for photovoltaics where the model has been tested in steady state time domain by doing various experiments. In our work, by changing the layer of thickness of MoO_3 and the active layer P3HT: PCBM (poly (3-hexylthiophene): phenyl-C61-butyric acid methyl ester) we have investigated the power conversion efficiency.

1.2. Statement of the Problems

One of the key challenges of organic solar cells is low power conversion efficiency. Main reasons behind low efficiency of organic solar cells include, limited photon absorption, difficulty in controlling morphology of an active layer, and charge carrier imbalance. Many researchers try to improve the performance of organic solar cell by modifying the morphology of the active layers by annealing at different temperatures and adding additive to the blend of active layer.

The other used different architecture of the devices to enhance the extraction of charge carriers for the performance improvement of organic solar cells. However, the investigations were not enough for commercialization of organic solar cells. Therefore, further improvement in power conversion efficiency requires detail investigations in the area to obtain the optimized parameters and architecture of the devices that boosts the performance of the cells. Limited literature on the use of various thickness of active layer for performance investigation of organic solar cells. Moreover, there are no reports using various active layer, HTL thickness and charge carrier mobility together to demonstrate the performance of organic solar cells. Therefore, in this work, the focus is to demonstrate the performance of inverted P3HT: PCBM based organic solar cell through optimizing the thickness of active layer, hole transport layer and electron mobility for the first time.

1.3. Significance of the Study

The energy demand has increased significantly due to the high consumption of electricity, elevation in the world population, and industrial dependency on electricity rather than fossil fuels. Energy has always played an important and inseparable role in civilization and human survival. Therefore, just stand alone source of energy is very important especially in scattered rural area of resident like Ethiopia. Solar energy is almost limitless. Sunlight provides by far the largest of all carbon-neutral energy sources. Organic solar cells have many advantages over inorganic solar cells. It is charging low prices to produce the materials and easy fabrication processes. They are also robust, flexible, and lightweight. However, the biggest challenges for successful commercialization of solar cells are the cells low efficiency and stability of the devices compared to inorganic photovoltaic cells. This study would proved a mechanism for improving the performance and stability of inverted organic solar cells through optimizing the active layer thickness, hole transport layer thickness and electron mobility.

1.4 Objective

1.4.1 General Objective

- The general objective of this work is to boost performance of P3HT: PCBM based an inverted bulk hetero junction organic solar cell by optimizing the morphology of active layer (P3HT: PCBM).

1.4.2. Specific Objectives

The specific objectives of this research are:

- To optimizing the thickness of active layer (P3HT: PCBM) and hole transport layer.
- To observe the effect of electron mobility on the performance of organic solar cells.
- To design the inverted BHJ organic solar cells with device structure of ITO/ZnO/P3HT: PCBM/MoO_3/Al.
- Recording the J–V features of the designed devices.

CHAPTER TWO

LITERATURE REVIEW

2.1 Solar Energy As-long Term Alternative

Solar energy is a significant renewable energy alternative available to mankind. The sun, an abundant source of energy, imparts 173K TW of power on earth every day. Therefore, it has a huge potential to supply the world's total energy demands. However, only less than 0.1 % of world total energy consumption comes from solar cell. Major obstacles for the rapid commercialization of these solar energy systems are the process of installations and high costs of manufacturing. Improvement of high power conversion efficiency solar cell systems with high durability can reduce these costs. Therefore, improving efficient, low cost, and durable solar cells remains one of the important goals in solar energy research(Sahare, 2016).

2.2 Advantages and disadvantage of solar cells

2.2.1 Advantages of Solar Cell

Renewable Energy Source

Among the many advantages of solar panels, the most crucial is that it is a fully renewable energy source. It can be used in any part of the world and is available at all times. Solar energy, unlike certain other forms of energy, cannot be depleted.

Reduces Electricity Bills

Since you will be meeting some of your energy needs with the electricity your solar system has generated, your energy bills will drop. How much you save on your bill will be dependent on the size of the solar system and your heat usage or electricity. Moreover, not only will you be saving on the electricity bill, but there is also a possibility to receive payments for the surplus energy that you export back to the grid through the Smart export guarantee.

Diverse Applications

Solar energy can be used for diverse purposes. You can generate electricity (photo voltaic) or heat (solar thermal). Solar energy can be used to produce electricity in areas without access to the energy grid, to distil water in regions with limited clean water supplies and to power satellites in space. Solar energy can also be integrated into the materials used for buildings. Not long ago Sharp introduced transparent solar energy windows.

Low Maintenance Costs

Solar energy systems generally don't require a lot of maintenance. You only need to keep them relatively clean, so cleaning them a couple of times per year will do the job.

Technology Development

Technology in the solar power industry is constantly advancing and improvements will intensify in the future. Innovations in quantum physics and nanotechnology can potentially increase the effectiveness of solar panels and double, or even triple, the electrical input of the solar power systems(Nick Gromicko, n.d.).

2.2.2 Disadvantages of Solar Cell

Cost

The initial cost of purchasing a solar system is fairly high. This includes paying for solar panels, wiring, inverter, batteries, and the installation. Nevertheless, solar technologies are constantly developing, so it is safe to assume that prices will go down in the future.

Weather-Dependent

Although solar energy can still be collected during cloudy and rainy days, the efficiency of the solar system drops. Solar panels are dependent on sunlight to effectively gather solar energy. Therefore, a few cloudy, rainy days can have a noticeable effect on the energy system. You should also take into account that solar energy cannot be collected during the night.

Solar energy storage is expensive

Solar energy has to be used right away, or it can be stored in large batteries. These batteries, used in off-the-grid solar systems, can be charged during the day so that the energy is used at night. This is a good solution for using solar energy all day long but it is also quite expensive. In most cases, it is smarter to just use solar energy during the day and take energy from the grid during the night (you can only do this if your system is connected to the grid). Luckily your energy demand is usually higher during the day so you can meet most of it with solar energy.

Uses a Lot of Space

The more electricity you want to produce, the more solar panels you will need, as you want to collect as much sunlight as possible. Solar photovoltaic panels require a lot of space and some

roofs are not big enough to fit the number of solar panels that you would like to have. An alternative is to install some of the panels in your yard but they need to have access to sunlight.
If you don't have the space for all the panels that you wanted, you can opt for installing fewer to still satisfy some of your energy needs.

Associated with Pollution

Although pollution related to solar energy systems is far less compared to other sources of energy; solar energy can be associated with pollution. Transportation and installation of solar systems have been associated with the emission of greenhouse gases. There are also some toxic materials and hazardous products used during the manufacturing process of solar photovoltaic systems, which can indirectly affect the environment. Nevertheless, solar energy pollutes far less than other alternative energy sources(Bagher et al., 2015).

2.3 Types of Solar Cells

Solar cells can be classified into first, second, third and fourth generation cells. First-generation solar cells are primarily crystalline silicon. Silicon (Si) is the second most abundant element in earth's crust (after oxygen). There are several types of silicon-based solar cells: single crystalline silicon, polycrystalline silicon, microcrystalline silicon, and amorphous silicon (a-Si). Current solar cell production and commercial use are dominated by crystalline silicon modules, which represent~90% of the market. Second-generation solar cells are single-junction devices that aim to use less material while maintaining the efficiencies of first-generation photovoltaics. Some types of Second generation cells are thin film solar cells that include amorphous silicon, CdTe and CIGS cells and are commercially significant in utility-scale photovoltaic power stations, building integrated photo voltaic or in small standalone power system. The third generation of solar cells includes a number of thin-film technologies often described as emerging photo voltaic—most of them have not yet been commercially applied and are still in the research or development phase. Dye-sensitized solar cells and organic photovoltaics are common example of third generation. The last is fourth-generation solar cell technology. This technology makes use of the combination of organic and inorganic materials, as a means to increase the efficiency and cost-effectiveness of solar cells. The fourth-generation solar cells are engineered at solar scale and are characterized by the flexibility of conducting polymer films and the stable nanostructures. The main advantage of fourth-generation solar cell over the other technologies is that the

combination of organic and inorganic substrates improves the harvesting of solar energy, thereby ensuring effective efficiency while also maintaining meaningful cost savings(Bagher et al., 2015).

2.4 Organic Solar Cells

An organic photovoltaic cell or organic solar cell is one type of solar cell that uses conductive organic polymers for light absorption and charge transport. Organic semiconductors are organic materials showing the typical behavior of semiconductors, i.e they are insulators whose conductivity can be increased by doping, illumination, doping heating, or other processes increasing the charge carrier density. These devices are relatively easy to fabricate, can also be processed on flexible substrates, however they have relatively low stability and conversion efficiencies(Kana, 2011).

Organic solar cells, convert light into electricity using Conjugated organic molecules. Conjugated polymers are commonly used for these solar cells. Their long chain delocalization through alternate double and single bonds helps in effective charge transport in the cell. Therefore, when light irradiates these molecules, electrons are excited and jump from highest occupied molecular orbital (HOMO) to lowest unoccupied molecular orbital (LUMO). The energy difference between the low energy HOMO and the high energy LUMO is called the optical band gap(Sahare, 2016). The principle of operation for an organic solar cell(OSC) device is based on the conversion of incident electromagnetic radiation(EMR) to electrical charges which may then be extracted at the electrodes(anode and cathode). There are a number of processes which occur in order to achieve this and the OSC architecture is an ensemble of planar layers engineered to carry out these processes as efficiently as possible. Essentially the OSC device layered structure is tailored to accommodate the so -called active layer. In generally the operation of an OSC is listed as follows:

Photon Absorption – Photoelectric process begins when incident light of suitable wavelength energies are absorbed. Lower energy photons are transmitted through as energy loss, while thermalization losses will occur for higher energy photons. Upon photon absorption, there is a generation of electron-hole pairs (excitons). These excitons, which have a binding energy up to 0.4 eV are not able to dissociate thermally and require an interface with an energy difference for dissociation to occur.

Exciton diffusion - An energy input greater than 0.4eV is needed for electron-hole dissociation. The acceptor / donor material interface presents such an energetic condition, where the offset supplies the energy needed to break the bond. The electron-holes have to diffuse to this interface. These lifetimes for these electron-holes are limited in organic semiconductors with a maximum diffusion length of less than 20nm, where recombination will occur beyond that, leading to energy loss.

Exciton dissociation - As mentioned above, only a fraction of the electron-holes that diffuse to the interface are dissociated. The product of the dissociation are free carriers, where the hole portion remains in the donor layer while the electron is 'accepted' into the acceptor. The efficiency of the dissociation is dependent on the probability of this process that can be affected by the drift of the built-in electric field and proximity of the exciton formation to the interface.

Free carrier transport – Once the charge carries separated, the free holes and electron will then be transported from the organic layers to the corresponding electrodes, driven by a built-in electric field that is generated by the difference in work function of the electrode. In addition, the energy band can be tuned by inter layers to achieve band alignment that further promotes charge carrier transport by reducing the recombination of charges.

Free carrier collection – Charge carriers that reach the electrode interface are collected and transferred to the electrical circuit. Like the energy alignment by the inter layers, matching the energy levels at the photoactive / electrode layer interface improves the efficiency of collection(*Investigation of Charge Transport Properties of MoO3 Recombination and Optical Buffer Layers in Organic and Perovskite Solar Cells*, 2018).

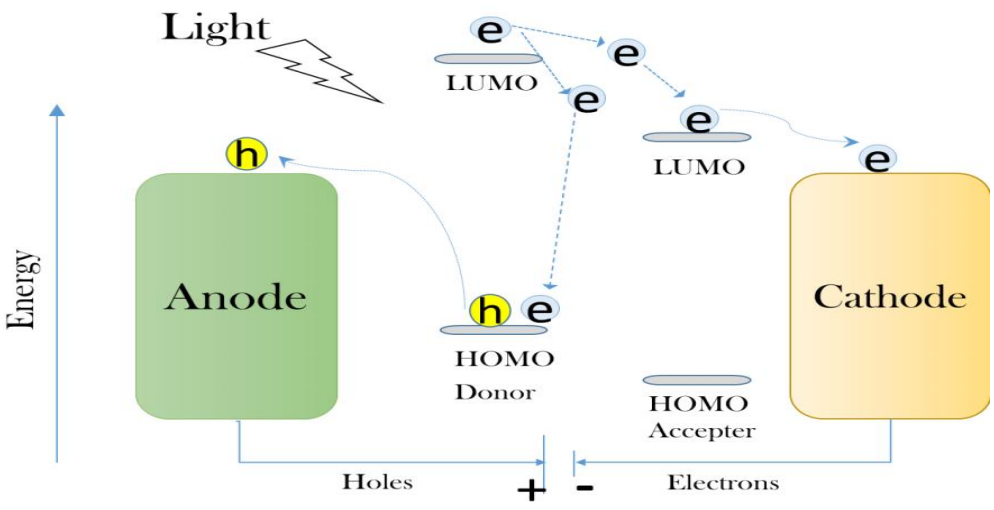


Figure 1 Working of an organic solar cell in schematic form(Sahare, 2016)

A typical organic solar cell is comprised of donor and acceptor molecules. The working of a typical organic solar cell can be better understood with the help of the schematic diagram shown in fig 1.

2.5 Some Organic Solar Cell Device Architectures

Typical organic solar cells are made of three layers, including a cathode, an anode, and an active layer. Active layer is kept in between the cathode and anode layers. However, one of the electrode should be transparent to light. Indium tin oxide (ITO) used as a transparent anode layer and a metal electrode such as calcium or aluminum used as a cathode layer. Organic Solar Cell devices are found in different device configurations such as single layer, bilayer, and blend. There has been much research done on device architectures of organic solar cells to enhance efficient charge transfer across the cell(Bagher et al., 2015).

2.5.1 Single Layer Organic Solar Cell

In earlier organic photovoltaic research, the first architecture proposed was the single layer organic solar cell. In this architecture, a photoactive organic layer is sandwiched between the anode and cathode. Indium tin oxide is used as a transparent hole collecting layer and aluminum or calcium as an electron collecting layer. The maximum power conversion efficiency achieved with these device architectures is, 0.1% (Sahare, 2016). The device architecture is shown in fig 2(Sahare, 2016)

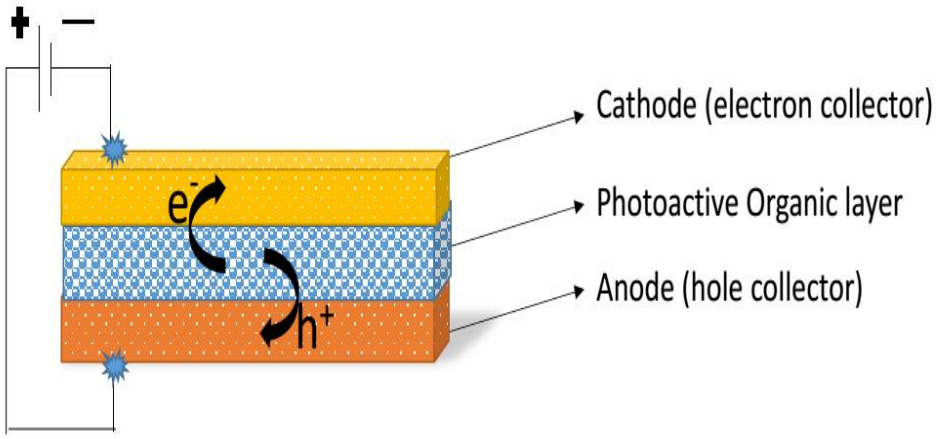


Figure 2 single layer device architecture(Sahare, 2016)

2.5.1 Double Layer Organic Solar Cell

This architecture was introduced to overcome the limitation of charge recombination in single layer organic solar cell. Double layer organic solar cells, as the name suggests, consist of two layers sandwiched between cathode and anode. Basically, the two layers are n-type electron acceptor and p-type electron donor. It enhances the functionality of the single layer organic solar cell by including a distinct organic donor layer and a distinct acceptor layer between the two previous electrodes. The drawback is the small interface that allows only excitons of a thin layer to reach it and get dissociated. A typical polymer layer needs a thickness of at least 100 nm to absorb enough light. At such a large thickness, only a small fraction of the excitons can reach the heterojunction interface, bearing in mind that the diffusion length of excitons is on the order of 4-10 nm(Kana, 2011).

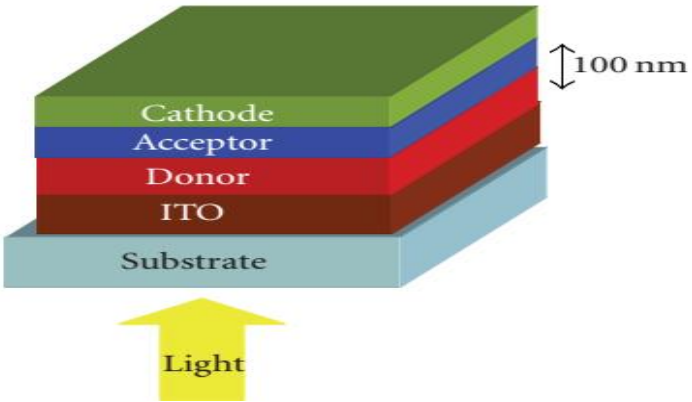


Figure 3 Two layer organic solar cell architecture(Kietzke, 2007)

2.5.3 Bulk Heterojunction (BHJ) Organic Solar Cell

This device architecture was proposed by Alan Heeger in 1995. In this architecture, a blend of donor and acceptor molecules is sandwiched between a cathode and an anode layer, making a network of donor-acceptor matrix. Instead of having distinct acceptor and distinct donor layers, in the blend layer solar cell device, the electron donor and acceptor are mixed together, forming a polymer blend. If the length scale of the blend is similar with the exciton diffusion length, most of the excitons generated in either material may reach the interface, where excitons break efficiently. The strong point of this type is the large interface area if the molecular mixing occurs on a scale that allows good contact between a like molecules (charge percolation) and most excitons to reach the donor or acceptor interface(Kana, 2011).

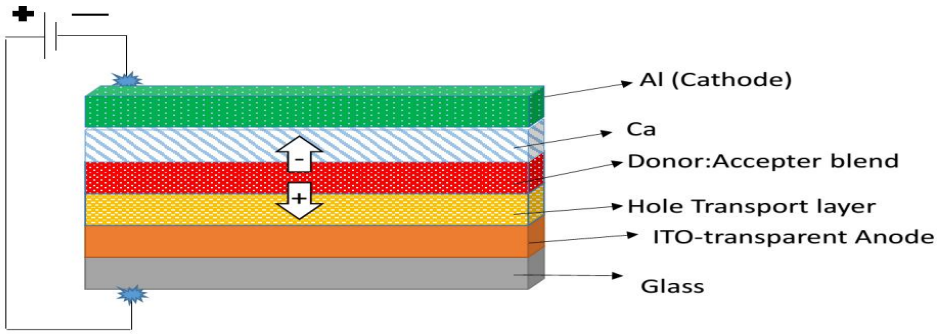


Figure 4 Normal BHJ organic solar cell(Sahare, 2016)

2.5.3.1 Inverted Bulk heterojunction (BHJ) Solar Cell

The inverted bulk heterojunction solar cell is an important modification to a typical single bulk heterojunction solar cell to improve the durability and stability. In this new architecture, an inverted geometry compared to the regular BHJ cell was developed. The device geometry is such that the charge carriers (electron and hole) move in the opposite direction when compared to the single BHJ solar cell. In a regular BHJ solar cell aluminum is used as a cathode, however, being a low work function metal it oxidizes in air. Here, the high work function metal such as silver is used to extract holes while the transparent ITO electrode is used to extract electrons from the active layer. Typically, a hole blocking layer(ETL) composed of Zinc oxide (ZnO) is placed in between the active layer and the transparent cathode, ITO, to hinder the charge recombination(Sahare, 2016). Fig 5 shows an Inverted bulk heterojunction solar cell(Sahare, 2016)

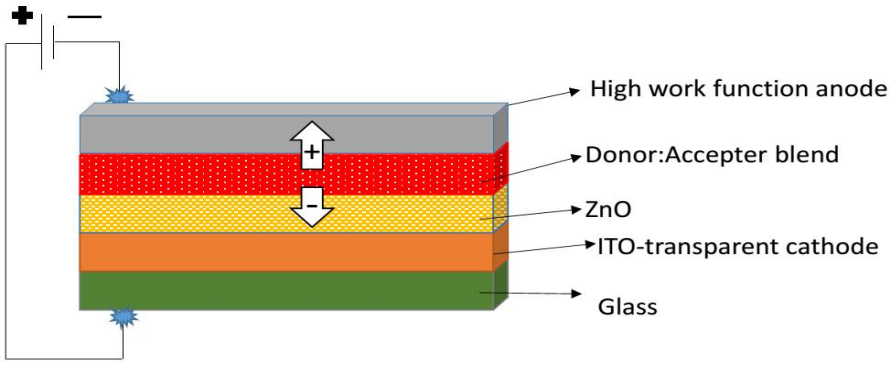


Figure 5 an Inverted bulk heterojunction solar cell(Sahare, 2016)

2.6 Photovoltaic Characteristics of a Solar Cell

The photovoltaic characteristics of a solar cell can be studied with a J-V plot which is obtained from measuring current with respect to the bias voltage. The photovoltaic parameters of a solar cell are fill factor, open circuit voltage, short circuit current density and power conversion efficiency (PCE). Fig 6 shows these parameters and an example of a J-V curve(Arbouch et al., 2014)

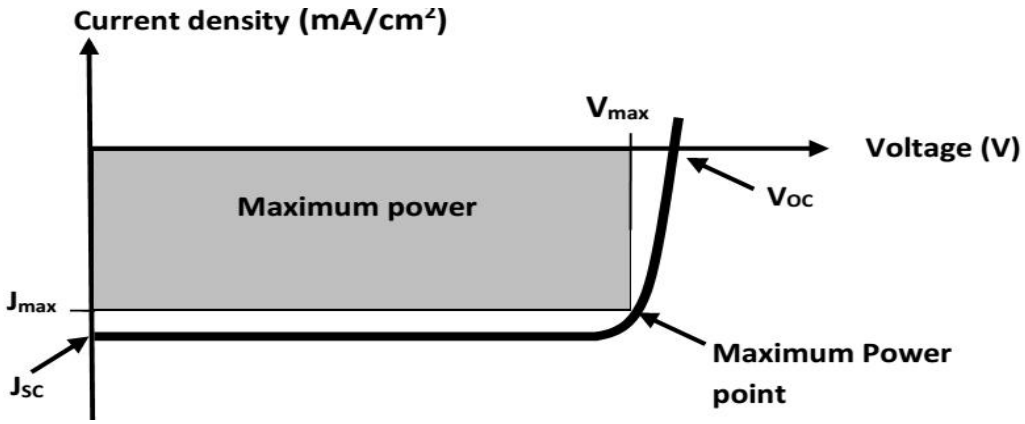


Figure 6 Current density vs Voltage(Arbouch et al., 2014)

2.6.1 Short Circuit Current Density (Jsc)

Short circuit current density is the maximum current (Imax) per unit area obtained from a cell when subjected to a short circuit connection. It is increases with increasing temperature. Taking short circuit current density as measure for the photo-current, this dependence can be attributed

to the thermal activation of polar on transport and exciton transport, probably along with temperature dependent exciton dissociation efficiency. Short circuit current density attributes to the efficiency of a solar cell due to light generated charge carriers. It depends on many factors such as the light intensity, area of the cell, collection probability by the electrodes, and spectrum of the incident light. The short-circuit current density (J_{SC}) at a specific wavelength was calculated as follows(Kempa et al., 2012):

$$J_{sc}(\lambda) = \text{EQE} \times (\text{spectral irradiance of AM1.5 G spectrum at } 1-\text{sun solar intensity}) \times \lambda/1.24 \quad 2.1$$

Where EQE is external quantum efficiency, λ is wavelength and $J_{sc}(\lambda)$ is short-circuit current density.

2.6.2 Open Circuit Voltage (Voc)

The voltage output obtained through the circuit at zero current value is the open circuit voltage. It depends upon the saturation current and current generated through radiation. It is directly associated with the band gap of the donor and acceptor molecules. Usually, the difference in energy level of the LUMO of a donor and the LUMO of an acceptor gives Voc for a particular blend. It has been observed that the value of open circuit voltage is directly proportional to change in band gap of donor and acceptor materials. The mathematical expression of Voc is given as follow.

$$V_{oc} = \frac{K_B T}{q} \ln\left(\frac{J_{ph}}{J_o} + 1\right) \approx \frac{K_B T}{q} \ln\left(\frac{J_{ph}}{J_o}\right) \quad 2.2$$

Where the approximation is justified because of $J_{ph} \gg J_o$

Equation 2.2 shows that Voc depends on the saturation current density of the solar cell and the photo-generated current. While J_{ph} typically has a small variation, the key effect is the saturation current, since this may vary by orders of magnitude. The saturation current density, Jo, depends on the recombination in the solar cell. Therefore, Voc is a measure of the amount of recombination in the device. Laboratory crystalline silicon solar cells have a Voc of up to 720 mV under the standard AM1.5 conditions, while commercial solar cells typically have Voc exceeding 600 mV.

2.6.3 Fill Factor (FF)

Fill factor (FF) is the ratio of maximum power from the solar cell to the product of a short circuit current and an open circuit voltage. This means that it determines the maximum power from the circuit in conjunction with the Isc and Voc. The magnitude of the square indicates higher power output. The fill factor is the ratio between the maximum power ($P_{max} = J_{mpp}V_{mpp}$) generated by a solar cell and the product of V_{oc} with J_{sc}.

$$FF = \frac{J_{mpp}V_{mpp}}{J_{sc}V_{oc}} \qquad 2.3$$

The subscript "mpp" in Eq. (2.3) denotes the maximum power point (MPP) of the solar cell, i.e. the point on the J-V characteristic of the solar cell, at which the solar cell has the maximal power output. To optimize the operation of PV systems, it is very important, to operate the solar cells (or PV modules) at the MPP. This is ensured with maximum power point tracking (MPPT).

2.6.4 Power Conversion Efficiency (PCE)

Power Conversion Efficiency (PCE) is the most important parameter of a solar cell that measures the performance and quality of the cell. It can be defined as the ratio of power output from the cell to the power input. In other words**,** power conversion efficiency is the ratio between the electrical energy achieved from the solar cell to light energy irradiated on the cell. The efficiency comparison between two different solar cells is based on the calibrated measurements performed under standard condition such as AM 1.5 and 1 sun intensity of light. The power input for power conversion efficiency, calculation was taken as 100 mw/cm^2 for one sun. Further, spectral mismatch should be avoided for accurate measurement of power conversion efficiency. Basically, the lamp used for photovoltaic study should have the same emission spectrum as that of the sun. PCE can be calculated by following formula

$$\eta = \frac{P_{max}}{I_{in}} x100\% = \frac{J_{mpp}V_{mpp}}{I_{in}} x100\% = \frac{J_{sc}V_{oc}FF}{I_{in}} x100\% \qquad 2.4$$

2.7 Improvement of Morphology

2.7.1 Solvent Annealing

Solvent annealing is a process in which the photoactive organic (donor-acceptor) layer is kept in a high concentration solvent environment. It was observed that solvent annealing can be used as

a treatment to control the morphology of the active layer film. Solvent annealing causes the polymer layer to swell, which further leads to reduction in the interparticle distance and improves crystalline order of the donor polymer layer. Crystallization due to solvent annealing causes the development of the interpenetrating network of donor-acceptor layers. This network usually diffuses through adjacent cathode layers, and provides percolated pathways to the charge carriers. This improved charge transfer mechanism results in increased power conversion efficiency. With this technique, the maximum efficiency achieved is 4.4%(Sahare, 2016).

2.7.2 Thermal Annealing

In thermal annealing, devices are placed at a certain temperature (T) for a certain period of time (t).Thermal annealing, similar to solvent annealing, has been proven to enhance the morphology of the polymer-fullerene blend. It can be done in two ways; pre- annealing and post- annealing. As the diffusion lengths of charge carriers are limited to 3 nm to 30 nm,(Peet et al., 2007) thermal annealing helps to increase the domain sizes of a blend. These domain sizes can be controlled with the annealing time and temperature.

Morphology control is very important in organic solar cells to obtain high efficiency solar cells. Although efficiency values have increased in last decay years, most of them have been achieved through trial and error, morphology control is still a challenge in organic solar cells. In an organic solar cell, when light strikes on active material, it creates excitons. These excitons have short diffusion lengths. Therefore, it is necessary to form an ordered structure of an active layer, to facilitate an easy transport of charge carriers. Charge carriers need percolated pathways to reach the oppositely charged electrodes and controlled morphology can improved by choice of solvent, inclusion of additives, regioregularity, ratio of donor and acceptor materials (Sahare, 2016).

2.7.3 Improve Photon Absorption

Compared to inorganic solar cells light absorption bands for organic solar cells are narrow. Most of the polymers and organic molecules do not absorb across the full solar spectrum. The most widely used donor polymer, poly (3-hexylthiophenes) (P3HT), absorbs only the red wavelength region of solar spectrum. This implies that, not all the incident light on organic solar cells converts light into photocurrent. This count to optical losses and one of the challenges to get higher power conversion efficiency. It is noticed that low band gap materials absorb a larger

spectrum of light. Therefore researchers have been working on development of novel narrow band gap materials.

Ideally, an incident photon should have an energy equivalent to the energy difference between the highest occupied molecular orbitals (HOMO) and lowest unoccupied molecular orbitals (LUMO) of the materials. However, when lower or higher energy photons fall on donor materials, a bound electron and hole with opposite spin are created. The columbic attraction between these charge carriers is higher than the work function difference between acceptor and donor molecules. Therefore, these charge carriers do not participate in band-to-band transition localization in the molecule itself. This results in loss of photocurrent in the cell(Cates et al., 2009).

2.7.4 Charge Carrier Imbalance

Charge carrier imbalance is a naturally occurring phenomenon with disordered morphology. As the exciton diffuses through the interface between acceptor and donor, it separates and moves as a charge carrier towards the oppositely charge electrode. However, due to absence of channels or percolated pathways for charge carriers, they get lost or recombined. It generates excess space charge in the donor-acceptor layer and reduces the performance of bulk hetrojunction solar cells. Usually, hole mobility across the electrodes is less than electron mobility; however, it was noticed that blending of PCBM with P3HT helped in balancing charge transport(Paul et al., 2007). It was also observed that thermal annealing and solvent annealing techniques drastically improves the hole mobility across the active layer. Improvement in crystallization during the annealing process is associated with an increase in hole mobility.

CHAPTER THREE
METHOD and MECHANISM

The methodology and mechanism used in this study were discussed in this section. The device is designed by using numerical software called general-purpose photovoltaic device model (GPVDM) and the physical mechanism of absorption explained extensively. In this research, a simulation on an inverted bulk hetero-junction device of ITO (Indium Tin Oxide, which is a transparent electrode): ZnO is used as ETL, P3HT: PCBM as active layer material, MoO_3 as HTL and Ag used as electrode was established by using a general-purpose photovoltaic device model (GPVDM) simulator at selected thickness of P3HT: PCBM and MoO_3 to obtain the J-V characteristic of the bulk hetero-junction device.

3.1. General-Purpose Photovoltaic Device Model (GPVDM)

GPVDM is a 1D/2D optoelectronic device model, which can be used to simulate solar cells, FETs, LEDs, diodes. This model is applied in this study for the simulation of optical and electrical properties. J-V graphs are plotted and obtain from the simulation results to reveal the pattern of the electron density when a voltage is applied to the stimulated device. Eq. (3.1) and Eq. (3.2) are applied to generate the J-V curve. The electrical simulation only covers for the active layer of the device as the main reaction occurs on the active layer of a device(Ismail et al., 2019).

$$I = I_o\left(e^{\frac{qv}{kt}} - 1\right) \quad 3.1$$

$$j_{external} = i_{ideal} + \frac{v_{applied}}{R_{shunt}} \quad 3.2$$

Where k is Boltzmann constant, I_o is the reverse saturation current, q is charge of electron, V is the applied voltage across the diode, t is temperature in Kelvin, i_{ideal} is ideal current, R_{shunt} is shunt resistance and $v_{applied}$ is applied voltage

3.2 Electrical Simulation

In this research work the electrical simulation has five different layers including the active layer. The layers from top to bottom ITO/ZnO/P3HT: PCBM/MoO_3/Ag is designed by using GPVDM.

This is an inverted BHJ solar cell has been done at different values of active layer thickness, hole transport layer thickness and electron mobility for one light intensity by using GPVDM Software.

In order to improve the efficiency of P3HT: PCBM based on an inverted organic solar cell, the main parameters that affect the performances of the OSC should be investigated. Indeed, numerical simulations under AM1.5 solar radiation for ITO/ZnO/P3HT: PCBM/MoO_3/Ag was demonstrated and the structure has been presented in fig 7 below by using GPVDM software to analyze the performance of the cell. The GPVDM software is based on the similar electrical model that is governed by the Poisson's equation, the continuity equations for electrons and holes, and the equations for drift-diffusion phenomena as follow(Meriem Erray, Hanine, Boufounas, & El Amrani, 2018; Islam et al., 2019).

Poisson's equation is given by-

$$\frac{d}{dx}\varepsilon_o\varepsilon_r\frac{d\varphi}{dx} = q(n-p) \qquad 3.3$$

Where ε_r is relative permittivity, ε_o is the permittivity of free space, ϕ is the voltage profile, n is the free electron concentration , q is the elementary charge of electron, and p is the free hole concentration. Equation (3.4) and (3.5) are the bipolar drift and diffusion equations for electrons and holes respectively(Farooq et al., 2019).

$$J_n = q\mu_e n\frac{\partial E}{\partial X} - qD_n\frac{\partial p}{\partial x} \qquad 3.4$$

$$J_p = q\mu_p p\frac{\partial E}{\partial x} - qD_p\frac{\partial p}{\partial x} \qquad 3.5$$

Where J_n is the electron current density, D_n is the electron diffusion coefficient, μ_e is the electron mobility, J_p is the hole current density, D_p is the hole diffusion coefficient, μp is the hole mobility, and E is electric field. Equation (3.6) and (3.7) are the electron and hole continuity equations in 1D and time domain (Farooq et al., 2019).

$$\frac{\partial J_n}{\partial x} = q\left(R_n - G + \frac{\partial n}{\partial t}\right) \qquad 3.6$$

$$\frac{\partial J_p}{\partial x} = -q\left(R_p - G + \frac{\partial p}{\partial t}\right) \qquad 3.7$$

Where, R_p is the net recombination rate for holes, R_n is the net recombination rate for electrons, and G is the free carrier generation rate. The 3-D graphical representation of the planner bulk hetero-junction architecture of our solar model is shown in figure-7. Here P3HT: PCBM is the

active layer. The layers configuration used in this simulation are respectively ITO/ZnO/P3HT: PCBM/MoO_3/Ag.

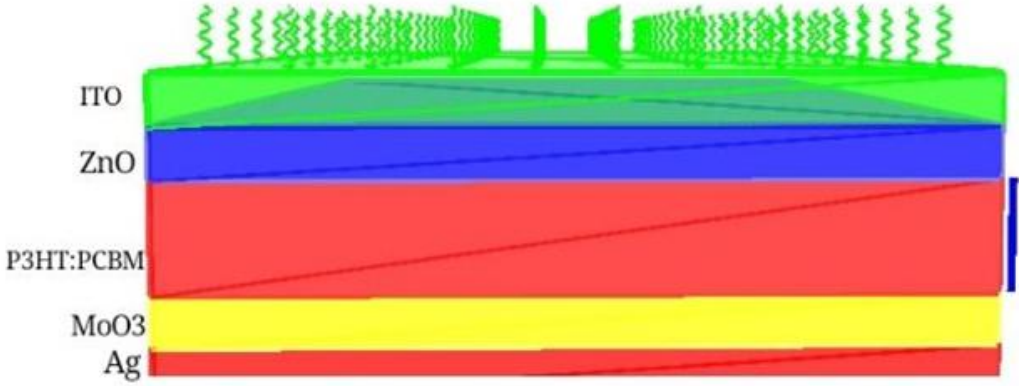


Figure 7 The3-D graphical representation of the planner bulk hetero-junction.

Here in fig.7, ITO (Indium Tin Oxide) is the oxide layer; ZnO is the oxides blending with P3HT: PCBM, MoO_3 is used as HTL and Ag is the metal layer. In the inverted organic solar cells standard structure, ITO substrate is the cathode and is coated with an electron transport layer (ETL), which is ZnO. On the top of ETL, is deposited a BHJ layer formed by a blend of n-type and p-type material (P3HT: PCBM). This layer is followed by an hole transport layer (HTL) often formed by a conductor oxide (MoO_3) and finally the anode which is silver (Ag). In our work, we have varied the active layer thickness, Hole transport layer thickness and the electron mobility. We first kept MoO_3 layer fixed at 5 different thicknesses and varied P3HT: PCBM layer under each thickness (case-I). Then again we kept P3HT: PCBM layer fixed at 4 different thicknesses and varied MoO_3 layer (case-II). Finally kept MoO_3 and P3HT: PCBM then varied electron mobility (case-III). For individual data sets, we have obtained PCE curves. The software was run for the following layer thickness to record the values of PCE, FF, Voc and Jsc.

Table 1: Simulation Parameter (for case I)

Layer Name	Layers Thickness(nm)
ITO	30
ZnO	20
P3HT:PCBM	140,180,200,220, 240
MoO_3	10

Ag	80

Table 2: Simulation Parameter (for case II)

Layer Name	Layers Thickness(nm)
ITO	30
ZnO	20
P3HT:PCBM	220
MoO_3	1,20,40, 60
Ag	80

In case III, to improve the device performance, one of the key parameter is charge carrier mobility and it should be optimized(M Erray, 2018). In our work we investigate how the device performance is affected by electron mobility. To see the effect of electron mobility from 50 $nm^2V^{-1}s^{-1}$ to 650 $nm^2V^{-1}s^{-1}$ on P3HT: PCBM.

Table 3: Parameters set for GPVDM Simulation(Abdallaoui et al., 2020; Sen & Bengal, 2019)

Parameters	**Value**
Electron trap density($m^{-3}eV^{-1}$)	$2x10^{26}$
Hole trap density($m^{-3}eV^{-1}$)	$2x10^{26}$
Electron mobility(m^2V^{-1} s^{-1})	$2.48x10^{-7}$
Hole mobility(m^2V^{-1} s^{-1})	$2.48x10^{-7}$
Trapped electron to free hole(m^{-2})	$1.32x10^{-22}$
Trapped hole to free electron(m^{-2})	$4.67x10^{-26}$
Free electron to trapped electron(m^{-2})	$2.5x10^{-20}$
Free hole to trapped hole(m^{-2})	$4.86x10^{-22}$

Using this numerical simulation different parameter such as Voc, Jsc, FF, PCE has been studied to understand the dependency of active layer thickness, hole transport layer thickness and electron mobility on device performance.

CHAPTER FOUR

RESULT and DISCUSSION

In order to optimize the thickness of the active layer, hole transport layer and electron mobility with special emphasis on improving the performance parameters with improved efficiency is main consideration. We have investigated a structure in which P3HT: PCBM is used as an absorber layers and effect of thickness on the performance of the cell is studied. In our proposed structure P3HT: PCBM is used as a main absorber material in which Ag and ITO is used on top and bottom electrode respectively. For hole transport layer and electron transport layer, MoO_3 layer and ZnO layer is utilized respectively.

4.1 The Effect of Active Layer Thickness

The dependence of active-layer thickness on the PCE of an inverted bulk hetro-junction organic solar cell based on P3HT: PCBM was investigated under this section. As the active-layer thickness increases, the number of absorbed photons is increases but the charge collection efficiency is expected to reduce because the recombination of charges. These two opposite changes determine the relation between PCE and active-layer thickness. This relationship has been theoretically and experimentally investigated by many researchers(Nakami et al., 2017). Layers stacked sequentially on top of each other in the inverted organic solar cells device, and the electrical and optical events such reflections at interfaces between layers and their interferences create a complex enhancement task with respect to the active layer thickness(Islam et al., 2019).

Therefore, the study of the active layer thickness is very significant since the thickness impacts the photon absorption and thereby the generation of holes-electron pairs inside the active layer(Abdallaoui et al., 2020). The effect of active layer thickness on the short-circuit current, open-circuit voltage, fill factor and power conversion efficiency of an inverted organic solar cell with ideal light trapping is described in this thesis work**.** To optimize the performance of P3HT: PCBM-based inverted organic solar cells; the active layer thickness has been varied from 140 nm to 240 nm. Figure 8 shows the J-V characteristics of the solar cell at different active layer thicknesses. The boosting of the power conversion efficiency in any type of solar cells is coupled to its parameters. These parameters are mainly: the Voc, Jsc, and FF. In general studies, a

common model P3HT: PCBM (only active layer) structure is used, but here, in case-I, we varied P3HT: PCBM (active layer) for different values of thickness i.e from 140 nm to 240 nm.

Fig 8 shows the graphical comparison among different active layer thickness and their effects on PCE. It can be seen from Figure 8 that when P3HT: PCBM layer is fixed at 220 nm, there is a sudden increase in PCE to 5.158%, but not so significant. Fig 8 is show the J-V curve at different thickness of active layer.

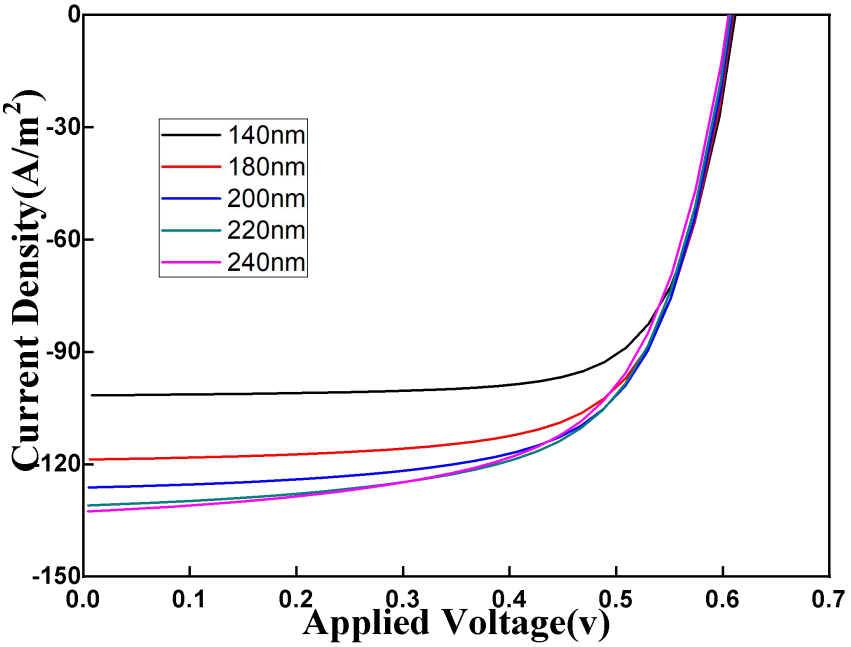


Figure 8 Current density v_s. Applied voltage.

Table 4: Evaluated parameters of the cells for various thickness of active layer

Active layer thickness (nm)	J_{sc}(A/m^2)	V_{oc}(V)	FF	PCE%
140	-101.5	0.612	0.729	4.533
180	-118.7	0.609	0.692	5.007
200	-126.2	0.608	0.668	5.137
220	-130.9	0.607	0.647	5.158
240	-132.5	0.605	0.668	5.067

Fig 8 shows the graphical comparison among different active layer thickness and their effects on PCE. We see from the Fig 8 that when P3HT: PCBM layer is fixed at 220 nm, there is a sudden increase in PCE to 5.158%, but not so significant. However, a detailed study of the effects that

active layer thickness has on the efficiency and short circuit current has not been performed for bulk hetero-junction polymer solar cells so far. We demonstrate that the performance of these devices is highly dependent on the active layer thickness and, using a well established model for optical and electrical interference, we show that such effects are responsible for the variations in performance as a function of active layer thickness. Fig 8 shows the thickness dependence of power conversion efficiency for inverted organic solar cell. In the case of our work inverted organic solar cell, the optimum thickness is around 220 nm, above which PCE gradually decreases with increasing active-layer thickness. This result is consistent with one report on inverted and some on conventional organic solar cells(Nakami et al., 2017). Finally, a device with an active layer thickness of 220 nm is designed with a power efficiency of 5.15% under AM1.5 illumination at intensity of 100 mW/cm^2. Fig 9 shows the J-V curve at active layer thickness of 220 nm as follow.

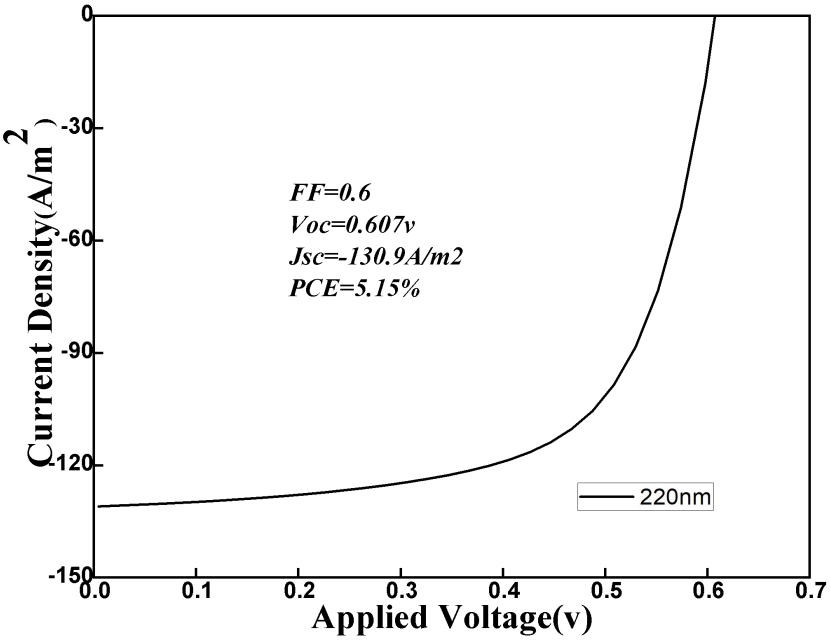


Figure 9 Current density v_s Applied voltage at AL thickness 220 nm

4.2. Effect of Hole Transport Layer (HTL) Thickness

Now, the HTL thickness effect is considered. The importance of buffer layers, that is HTL, is to act as electron blocking layers and to enhance carrier collection in the device. In this part, the HTL thickness dependent effect on the performance of an inverted organic solar cell is undertaken. The hole transport layer commonly known as the buffer layer is used to increase carrier collection in cells(Sen & Islam, 2018). This study shows the dependence of the

performance of simulated inverted OSC on the variation in HTL thickness. The photoactive layer P3HT: PCBM is fixed at the optimized thickness of 220 nm.

The HTL material between the front anode (Ag) and the photoactive layer (P3HT: PCBM) should favor the electron conduction and restrict the transport of electron toward the anode, thereby, preventing the recombination of charge carriers near the anode. In this section, the variation of hole transport layer thickness is investigated through GPVDM simulations. Molybdenum Oxide (MoO_3) is chosen as hole transport layer due to its concomitant properties like high conductivity, better transparency, and better hole transportation (Gupta et al., 2022). The MoO_3 thickness is varied between 1-60 nm. The J-V characteristic curves and other parameters obtained through the simulations are drawn in Fig 10. As seen in Fig 10, the variation in HTL thickness has no prominent effect on FF and V_{OC}, which is due to the low electron mobility.

The optimized inverted organic solar cell is obtained at 20 nm thickness of HTL. Jsc, and PCE slightly vary with variation in the thickness of HTL and exhibit the optimum values at 20 nm. Voc and FF remain almost insensitive to variation in thickness of hole transport layer. Consequently, the thickness of hole transport layer has a minor effect on electrical parameters of simulated inverted organic solar cell due to the low hole mobility. The best performance is obtained at 20 nm HTL thicknesses. Furthermore, as the HTL thickness increases, slight decrease is observed in Jsc and PCE, in agreement with (Li et al., 2017). Fig 10 shows the graphical comparison among different holes transparent layer thickness and their effects on PCE.

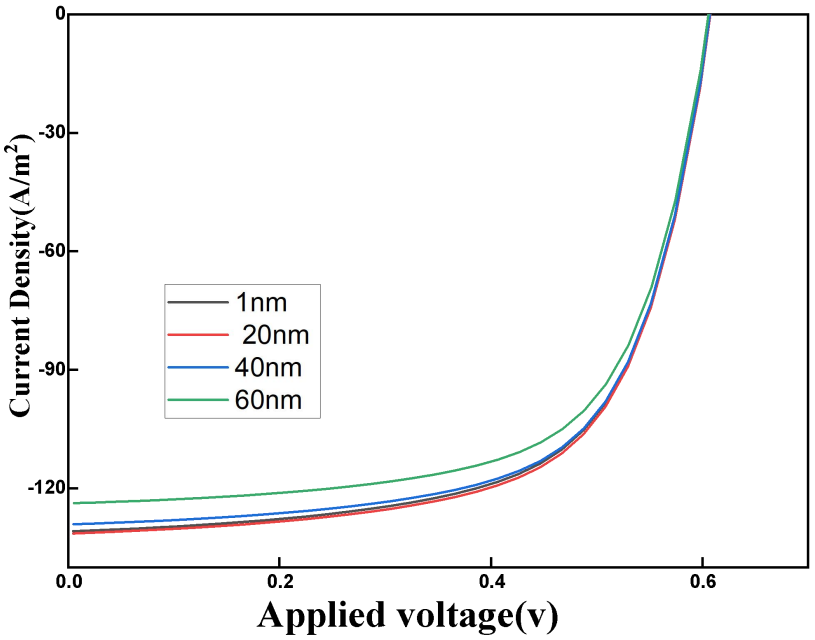


Figure 10 Current density v_s Applied voltage at different thickness of HTL

We observe the parameters like J_{sc}, V_{oc}, FF& PCE from the fig 10; the values are given as follow.

Table 5: Evaluated Parameters of the Cells for Various Thickness of HTL

HTL thickness (nm)	$J_{sc}(A/m^2)$	$V_{oc}(V)$	FF	PCE%
1	-130.89	0.607	0.647	5.147
20	-131.44	0.6075	0.65	5.192
40	-129.3	0.6072	0.653	5.122
60	-123.56	0.6058	0.655	4.91

The above table-5 indicates that at the thickness of HTL (MoO_3) is 20 nm, the highest power conversion efficiency is obtained which is the value is 5.192%. As seen in Fig 10 and table 5, the variation in HTL thickness has no dramatic effect on FF and V_{OC}, which is due to the low hole mobility. The optimized inverted organic solar cell is obtained at 20 nm thickness of hole transport layer. J_{sc} and PCE slightly vary with variation in the thickness of hole transport layer and exhibit the optimum values at 20 nm, the highest PCE is obtained which is the value is 5.192%. FF and Voc remain almost insensitive to variation in thickness of hole transport layer. Consequently, the thickness of hole transport layer has a minor effect on electrical parameters of simulated inverted organic solar cell due to the low hole mobility(Sen & Islam, 2018)

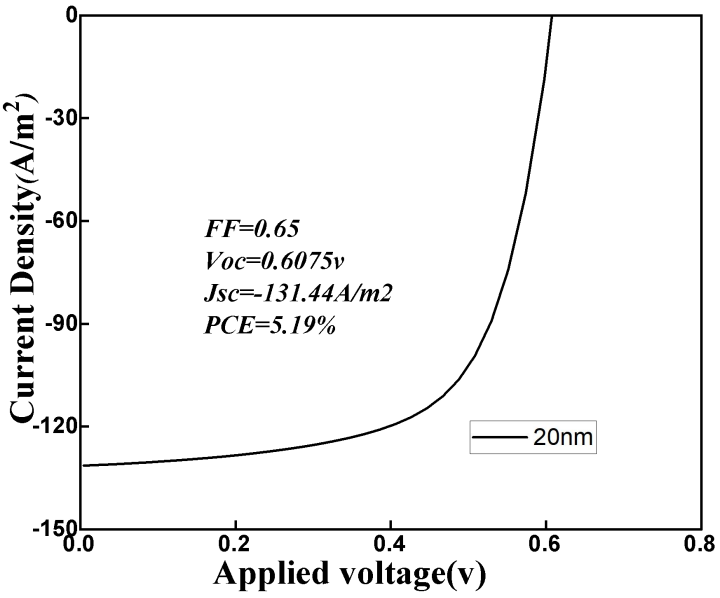


Figure 11 Current density v_s Applied voltage at the HTL thickness of 20 nm.

4.3. Effect of Electron Mobility

Now, the electron mobility effect is considered. Hole transport layer and active layer thicknesses are fixed at 20 nm and 220 nm respectively. Electron mobility is another mechanism to enhance the efficiency of solar cells and it should be optimized. The electron mobility is an important parameter for inverted organic solar cell materials as it influences the recombination dynamics and charge extraction. In this thesis work, the GPVDM simulation is used to investigate the electron mobility of the important organic photovoltaic materials P3HT, PCBM and their blend. It is characterizes how quickly an electron can move through a semiconductor or a metal when pulled by electric field. In order for there to current, the holes and electrons must move. The ability for them to move around in a transport charge and material is called mobility, there's electron and hole mobility. These are not necessarily constants inherent to holes and electrons. Several factors affect the mobility of a carrier. The most significant is the motion-impending collisions within the crystal and scattering. These collisions can be an electron bumping into another hole, or an electron or ionized impurities. Scattering may decrease /increase due to temperature and the addition of donors or acceptors. The more excited the carriers are, the more scattering there will be at higher temperatures(Sen & Bengal, 2019).

In order to enhance the performance of inverted organic solar cells, it is necessary to collect a maximum number of generated charge carriers. This thesis work is not only investigates how the device performance is affected by the thickness of active layer and hole transport layer , but also the effect of electron mobility is investigated. In case-III to see the effect of electron mobility on the performancee of P3HT: PCBM based on an inverted bulk organic solar cells , electron mobility is investigated in the range of 10^{-4} cm^2V^{-1} s^{-1} to $3.2x10^3$ cm^2V^{-1} s^{-1}, based on the different works reported(Meriem Erray, Hanine, Boufounas, & Amrani, 2018; Sen & Bengal, 2019) . In this work we use Layer thickness of ITO, ZnO, P3HT: PCBM, MoO_3 and Ag have been used as 20 nm, 10 nm, 220 nm, 20 nm and 80 nm respectively and then vary the electron mobility from 50 $nm^2v^{-1}S^{-1}$ to 650 nm^2 $V^{-1}S^{-1}$. Using this numerical simulation different parameter such as J_{sc}, V_{oc}, FF and PCE has been studied to understand the dependency of electron mobility on device performance.

As noticed from fig 12, short circuit current density (J_{sc}) is found to decrease with electron mobility which is due to the loss in free charges n and p due to the Langevin recombination which increases with charge mobility, this is in good agreement with equation 4.1 (Sen & Bengal, 2019).

$$R_D = \frac{e(\mu_n+\mu_p)}{\varepsilon_o\varepsilon_r}(np - n_o p_o) \qquad 4.1$$

Fig 13 shows the variation of open circuit voltage (V_{oc}) with electron mobility and it is found to slightly decrease with electron mobility. Fill factor v_s. electron mobility has been found to vary in similar manner as shown in following fig 14. Efficiency is found to increase with electron mobility up to $4.5x10^{-7}m^2$ V^{-1} S^{-1} and then it becomes constant at nearly 5.16%. Fig 15 shows the relationship between efficiency and electron mobility.

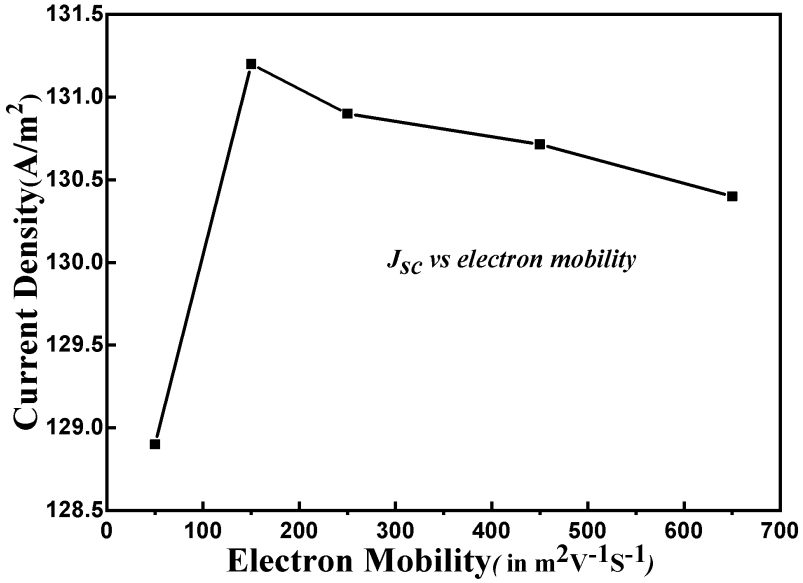


Figure 12 Short circuit current density vs. Electron mobility

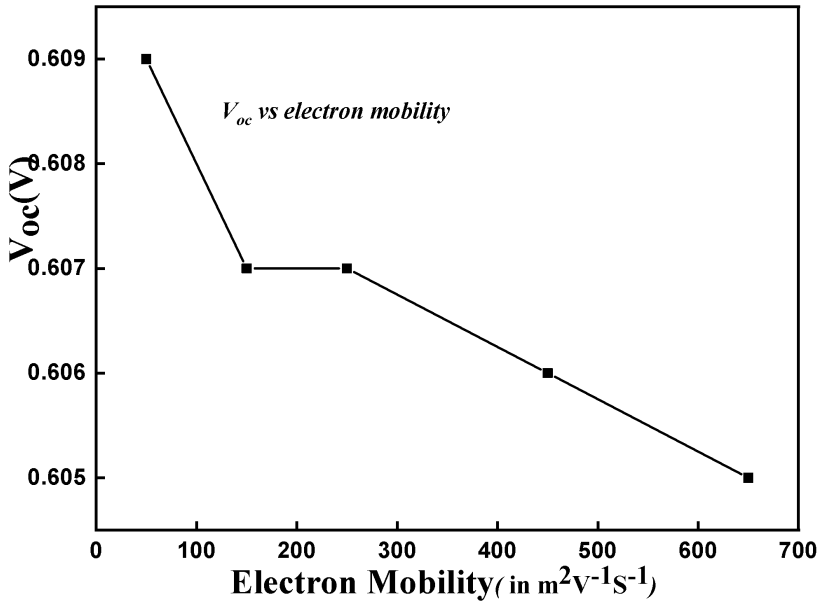


Figure 13 Open circuit voltage vs. electron mobility

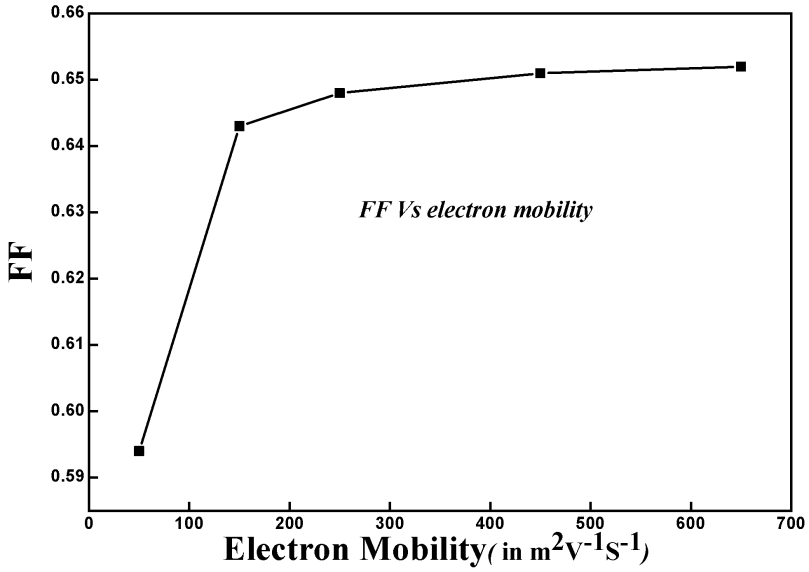


Figure 14 FF v_s electron mobility

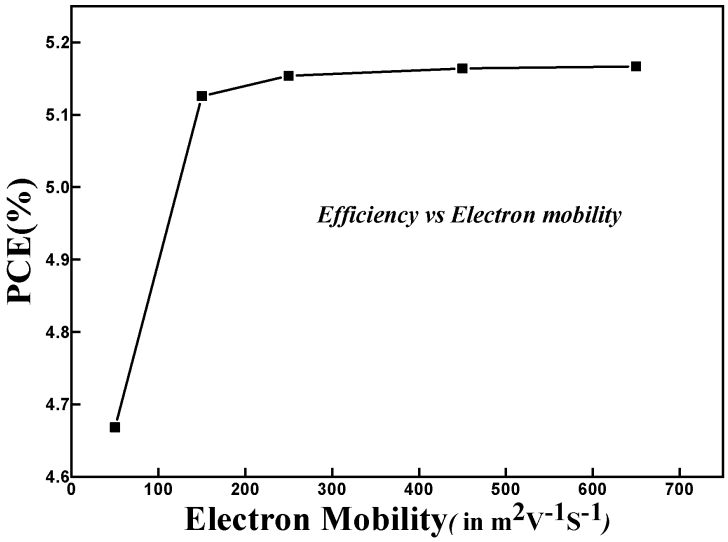


Figure 15 Efficiency v_s electron mobility

The energy level diagram of the device structure is explained as follow in fig 16. Energy level alignment at donor -acceptor hetero-junctions is very important for understanding the charge recombination and generation process in inverted organic photovoltaic devices.

However, the energy level alignment at the donor-acceptor interfaces is largely underdetermined; resulting in debates on the fundamental operating mechanisms of high-efficiency non-fullerene inverted organic solar cells. Here, we systematically investigate energy level alignment and its depth-dependent variation of a range of donor -acceptor interfaces by fabricating donor -acceptor quasi bilayers and planar bilayers.

Schematic energy level diagram for P3HT: PCBM blend of inverted organic solar cells with ITO/ Ag and Zno/MoO_3 as electrodes and charge transport layer respectively. The hole-electron pair is generated by one sun light in a blend of P3HT and PCBM, where P3HT acts as an electron donor and PCBM acts as an electron acceptor and provides interface and work function energy for charge separation.

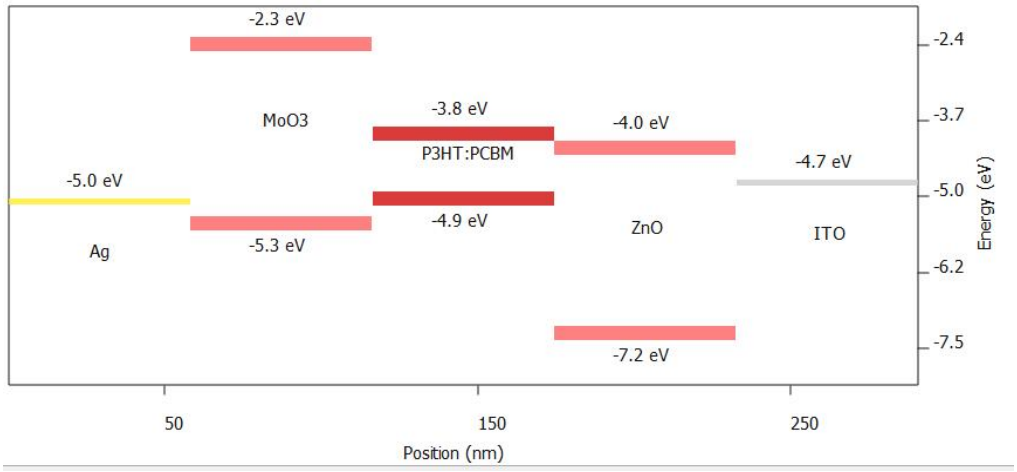


Figure 16 The energy level diagram of the device structure

Distribution of photon density based on visible light wavelength is explained as the follow fig 17. In order to investigate the photon distribution in optoelectronic devices, the simulation software GPVDM was used. For optimization of the transport layer thicknesses, the electron mobility and the absorptivity of the absorption layer was maximized for the AM1.5 solar spectrum. The energy of a photon is directly proportional to its frequency and inversely proportional to its wavelength. Thus as frequency increases, the photon energy increases and visa versa. Photon density is similar to intensity, but it needs to take into account the number of photons in a specific volume at any given time.

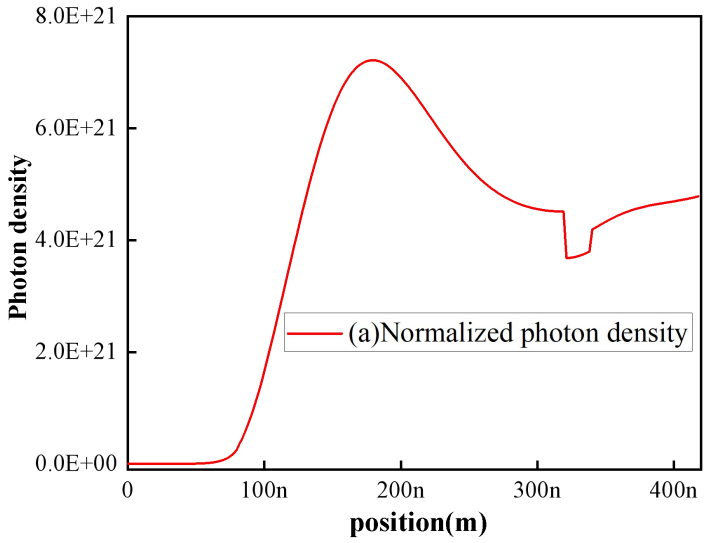
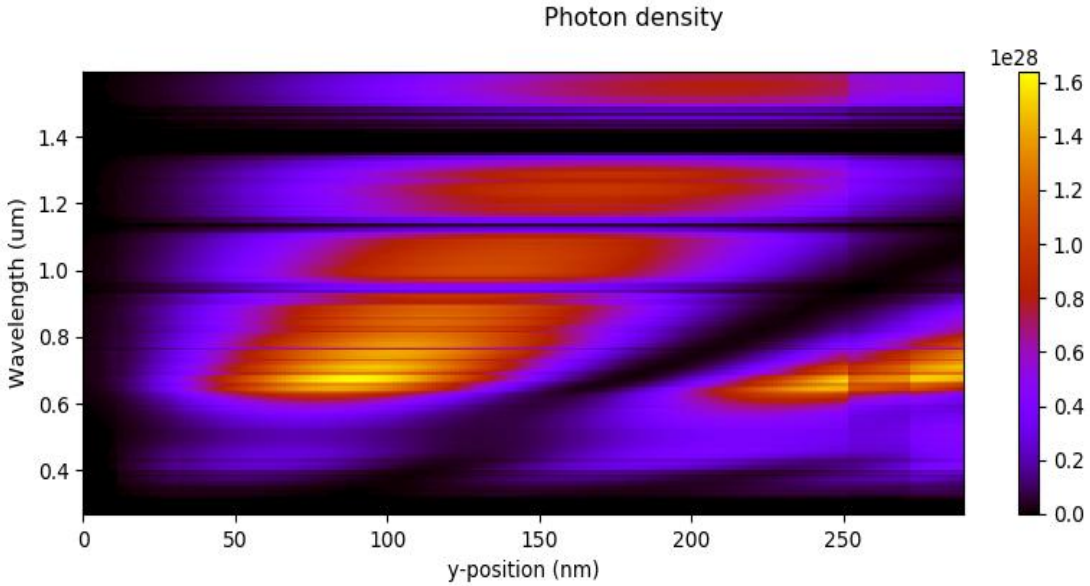


Figure 17 Normalized photon density



(b)

Figure 18 Distribution of photon density based on visible light wavelength.

Absorbed photon density in different components of the device architecture of ITO/ZnO/ P3HT: PCBM/ MoO_3 /Ag shows as Fig. 18 below. It is visible from the graph that the absorption is increases from 0 nm to 250 nm in which absorber material is positioned. It also shows

distribution of photons in the different material of the cell, and it's visible from the figure that the photons are distributed randomly from 400 nm wavelength to 1400 nm wavelength.

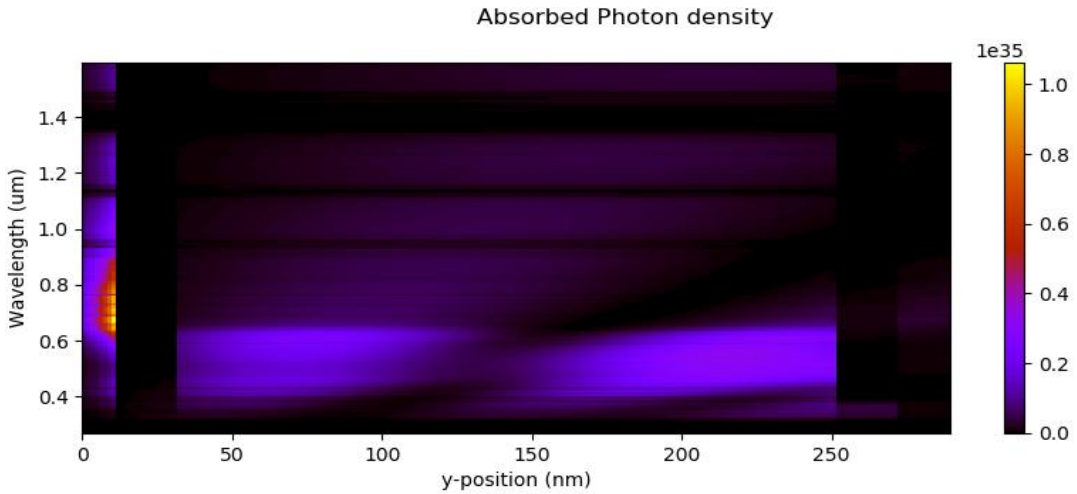
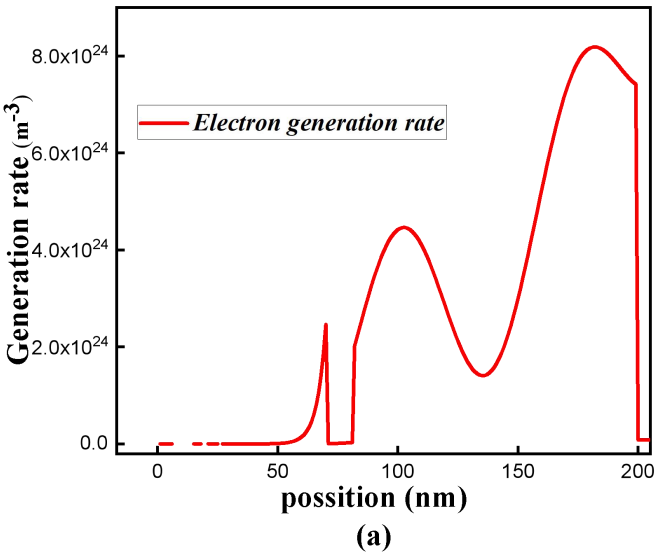


Figure 19 Absorbance of the device.



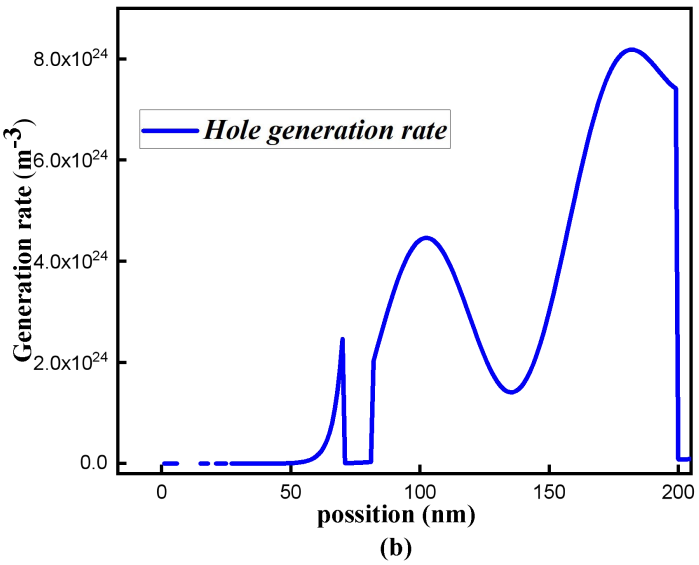


Figure 20 Generation rate of (a) electron and (b) hole for ITO/ZnO/ P3HT: PCBM/ZnO/Ag device architecture.

Electron and hole generation rate as the position of device components have been demonstrated and shown in Figures 19(a) and 19(b), respectively. Accordingly, both charge carriers' generation rates are high in the bulk heterojunction blend of donor and acceptor. Thus, the inverted bulk heterojunction used as an active layer plays a major role in organic solar cell efficiency optimization.

CHAPTER FIVE

5. CONCLUSION and RECOMMENDATION

5.1 Conclusion

The performance of inverted P3HT: PCBM based organic solar cell with the structure of ITO/ZnO/ P3HT: PCBM/ZnO/Ag has been investigated. The effect of active layer thickness, hole transport layer thickness and electron mobility has been studied separately using simulating software GPVDM. With constant HTL thickness and electron mobility, the power conversion efficiency of the device at various thickness of active layers demonstrated and obtained 5.158% maximum PCE at 220 nm active layer thickness. For fixed thickness of active layer and electron mobility, the demonstration result for various HTL thickness shows a slightly increases of the efficiency to 5.193% at 20 nm of the thickness hole transport layer. From electron mobility variation, 5.23% efficiency can be achieved at electron mobility of $4.5x10^{-7}m^2\ V^{-1}\ S^{-1}$ for the fixed thickness of active layer and HTL. Investigation results show that thickness of active layer, hole transport layer and electron mobility play important role to optimize the performance of the P3HT: PCBM based organic solar cell. Thus to enhance an inverted organic solar cells performance, the thickness active layer, hole transport layer and electron mobility has to be optimized.

5.2 Recommendation

Energy has always played an important and inseparable role in civilization and human survival. Therefore, just stand alone source of energy is very important especially in scattered rural area of resident like Ethiopia. Solar energy is almost limitless. Sunlight provides by far the largest of all carbon-neutral energy sources. Among many types solar cells, organic solar cell has many advantages than other types. It is charging low prices to produce the materials and easy fabrication processes. They are also robust, flexible, and lightweight. From this thesis work we understand the efficiency of an inverted organic solar cell is affected by active layer thickness, hole transport layer thickness and the electron mobility and optimize them by using GPVDM soft ware. We recommended for future during fabricating the device it is better to use the thickness of active layer (P3HT : PCBM) , hole transport layer thickness (MoO_3) and electron mobility 220 nm, 20 nm and $4.5x10^{-7}m^2\ V^{-1}\ S^{-1}$ respectively to obtain high efficiency.

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