

Enhanced Organic Photovoltaics (EOPV):

A theoretical model of a polymer based efficient solar cell

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Abstract-

Solar energy is renewable, eco-friendly and found in abundance. If optimized properly, it can fulfill the energy requirements of contemporary world. At present, the efficiency of Silicon based solar cells lies between 10-15% and also it is not cost effective. Due to certain limitations of Si-based solar cells researchers are moving towards an alternative i.e. Organic Semiconductors. Organic Semiconductors possess properties like good electrical conductivity, mechanical strength, optical absorption, photoluminescence, easy and cheap manufacturing etc. In this paper, we aim to design a solar cell that intercepts most of the energy spectrum of sunlight and converts it into electricity efficiently. After having a detailed study of latest researches and analyzing the properties of many substances, we created a theoretical model of polymer based solar cell. The model uses aluminum studs at the interface and Bulk-Heterojunction of Single Walled Carbon Nanotubes (SWCNTs) and Organic polymer- Poly Butylene Terephthalate (OP-PBT) as an electron donor and acceptor respectively. We will explain how our model –EOPV intercepts and interacts with the photons of different wavelengths and how these photons penetrate and produce ‘excitons’ which in turn generates photocurrent. Based on certain assumptions and calculations our EOPV model exhibits the efficiency of more than 40% which is comparatively better than existing conventional models.

Keywords- Enhanced Organic Photovoltaics (EOPV), Organic Semiconductors, Aluminum studs, Bulk Heterojunction, Single Walled Carbon Nanotubes (SWCNT), Organic Polymer- Poly Butylene Terephthalate (OP-PBT), Excitons, Photocurrent.

I. Introduction

Solar energy is the basic source of energy on earth. We receive solar energy in the form of sunlight. The power density received from the sun at sea level is about 1 kW/m². If we can efficiently tap the solar energy, it can fulfill all our energy requirements. This is the reason why in the recent years, there has been a lot of researches and development in the field of solar cells. Photoelectric theory is the basis of converting solar energy (in the form of photons) into electricity. When light shines on the solar cell, photons collides with the electrons and it jumps from the valence band to the conduction band generating electron-hole pair. And when these electron-hole pairs are collected separately photocurrent is generated. In order to improve the Power Conversion Efficiency (PCE) of the solar cell we have to design a system that utilizes most of

the solar energy spectrum and converts it into electricity efficiently. The conventional solar cells, which are basically Silicon based, intercepts only Infrared portion of Electromagnetic energy spectrum. Another disadvantage of Silicon based solar cell is that it is costly, heavy, non-flexible and causes transportation problem. This is the reason why solar cells are not gaining enough popularity among common people. In order to make it cost effective, flexible and efficient, researchers are moving towards an alternative i.e. Polymer based solar cells or Organic Photovoltaics (OPV). These are easy to handle and cheap. The major problem with OPV is its efficiency that lies between 7-10%. In order to improve the efficiency of Organic Photovoltaics our research team designed a model project that utilises Single Walled Carbon Nanotubes (SWCNTs) and Organic polymer- Poly Butylene Terephthalate (OP-PBT). We worked on the design of model, compatibility and stability of

the materials used and lastly found if fabricated properly, EOPV will yield good efficiency.

II. Traditional and Organic Photovoltaics: A Comparison

A. Traditional

Conventional solar cells are usually made from silicon *pn*-junction. The *n*-type silicon has extra, loosely bound electrons that can be ionized by the absorption of a photon leaving behind a hole. If this process occurs sufficiently close to the junction, then the electric field across the junction will pull the hole to the *p*-side. When an electrical contact is made between the two sides of the junction, electrons will flow from the *n*-side to the *p*-side, generating a current. However, the fact that the separated charges need to reach the junction before recombining limits these devices. Silicon is not the ideal material because it is a minority carrier. Meaning, the charge carriers are generated where they are outnumbered by opposite charges. Silicon was initially chosen only because it could build off the mature semiconductor industry. This problem has been mitigated by improving the purity and crystallinity of the silicon, which increases the distance travelled before recombination, and by creating multi-junction devices, which decreases the distance to the junction. Using these improvements, up to 35% of the photons can be converted to electrons. Nevertheless, these improvements greatly increase the cost of the solar cells, and without fundamental breakthroughs, silicon will not fulfil our Solar Energy's optimisation goal.

B. Organic

The cost of these devices will be much lower than traditional solar cells because they employ cheaper materials, such as conductive polymers, and processing techniques, such as spin casting and evaporation. There are generally three components in an organic solar cell: the active layer, band alignment layers and the electrodes. The active layer is the most important component. It composed of an electron donor and an electron acceptor and is responsible for photon absorption, charge separation and conduction to the electrode. The band alignment layers are placed between the active layer and the electrodes. Their role is to minimize the band bending that arises from the Schottky barrier between the semiconducting active layer and the metallic electrodes. Commonly, LiF is used on the Al

electrode and Poly (3, 4-Ethylene Dioxythiophene) PEDOT is used on the Indium Tin Oxide (ITO) electrode. The purpose of the electrodes is to serve as efficient charge collectors and to create an electric field throughout the active layer through the difference in their work functions. Usually Indium Tin Oxide (ITO) is chosen because it is transparent and has a high work function (4.7 eV). It usually paired with Aluminium (4.28 eV) because they have a large difference in work function (0.4 eV).

In Organic photovoltaic function there are essentially four steps from photon to electron conversion: photon absorption, excitons diffusion to junction, charge separation, and charge transport to their respective electrodes. But the major challenge is the interface recombination of excitons.

III. Enhanced Organic Photovoltaics (EOPV): A Theoretical Model

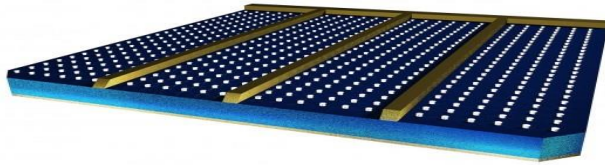
A. Objectives

Our research team endeavoured to design a polymer based solar cell model that absorbs maximum sunlight, intercepts most of the solar energy spectrum and converts it into electricity with a maximum efficiency. We also focused on the fact that materials used must be easily available to the manufacturers. So based on the necessities we deeply studied materials and selected some of them which possess the required properties.

B. Materials used

i. Aluminium studs

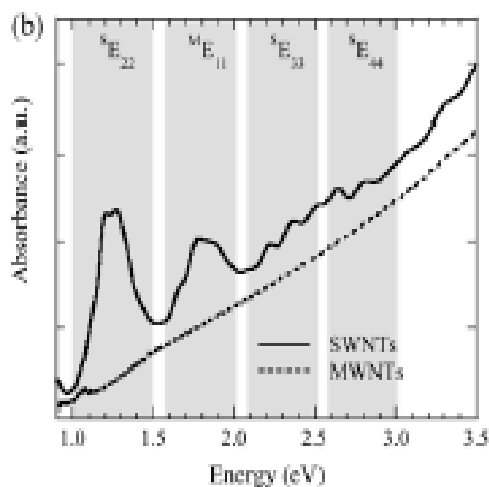
An array of cylindrical aluminum studs on top of a solar cell can dramatically improve the amount of light trapped inside its absorbing layer. In most solar cells, about half of the manufacturing costs are taken up by the absorbing layer alone. This all-important layer is where incoming photons collide with the atoms in the structure and "knock off". Besides being cheaper and more abundant, aluminum is also much better at reflecting and scattering light without absorbing it. Thus, when photons hit the nano-array, many more are deflected and travel through the absorption region for greater distances, as originally intended.



(Figure 1: Aluminium studs image by Imperial college of London)

ii. Carbon Nanotubes (CNTs)

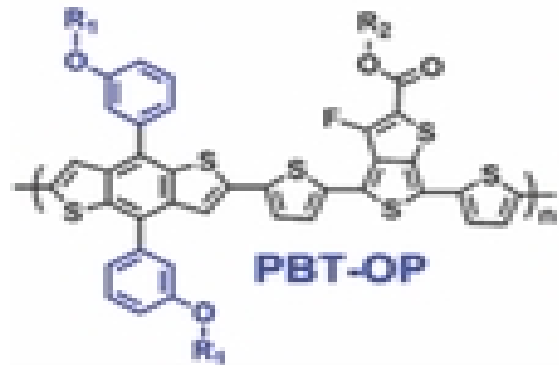
CNTs has high optical absorbance (needed to produce excitons) and extremely high conductivity (needed to move the charges to the electrodes). There are two types of CNTs, Single walled nanotubes (SWNT) and Multi walled nanotubes (MWNT). But SWNT have much higher absorbance spectra peaks than in MWNT.



(Figure 2: Comparison of the optical absorbance spectrums for SWCNT and MWCNT)

iii. Organic Polymer- Poly Butylene Terephthalate (OP-PBT)

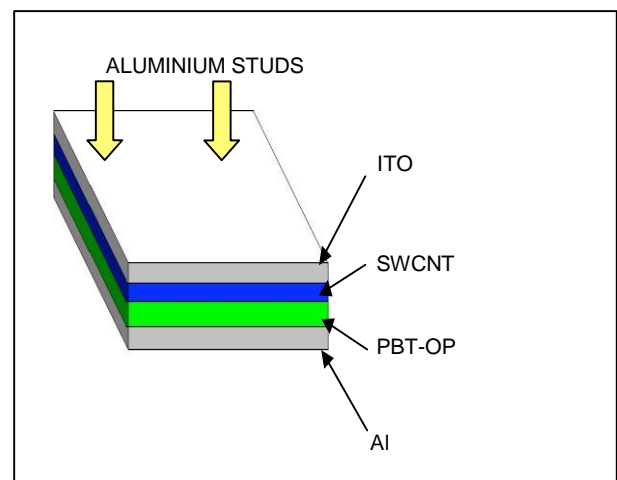
OP-PBT is manufactured from one easily synthesized monomer and two commercially available monomers. OP-PBT is not only easier to make than other commonly used polymers, but a simple manipulation of its chemical structure gave it a lower HOMO (Highest Occupied Molecular Orbital) level than had been seen in other polymers with the same molecular backbone because of the presence of fluorine. OP-PBT showed an open circuit voltage (the voltage available from a solar cell) value of 0.78 volts, a 36 percent increase over the ~ 0.6 volt average from similar polymers, Fill Factor (FF) of 71.8% and Current Density (J_{sc}) of 13.4mA/cm².



(Figure 3: Molecular structure of OP-PBT)

C. Model of Enhanced Organic Photovoltaics (EOPV)

At the interface we have embedded nano-cylindrical Aluminum studs upon the electrode ITO. Bulk Hetrojunction of SWCNT and OP-PBT is sandwiched between electrodes ITO (Anode) and Al (Cathode).



(Figure 4: Model of EOPV)

IV. Working of Enhanced Organic Photovoltaics (EOPV)

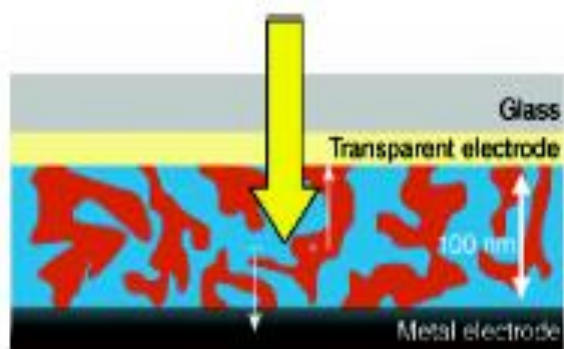
A. Photon Absorption

In this model, we designed Aluminium studs on the interface which directs a lot of photons to the absorption region. The photon absorption usually occurs in the electron donor, although both donor and acceptor can absorb. The key material property related to photon absorption is absorption coefficient. While conductive polymers can have very high absorption coefficients, they tend to be only for low wavelengths (300-400 nm)

which do not match the solar spectrum very well. This means that for adequate photon absorption to occur, the thickness of the active layer needs to be increased. This is undesirable because it increases the distance that separated charges need to be transported and lowers the amount of charges that reach their electrodes. We hope that by using SWCNTs as the electron donor, we can increase the absorption efficiency of the cell.

2. Excitons Diffusion to Junction

Photon absorption creates excitons which are electron-hole pairs that are bound to each other via Coulombic attraction. In order to generate charges, these electron-hole pairs must be separated at a donor/acceptor junction before they recombine. Unfortunately, due to short excitons' lifetime and poor mobility conductive polymers have very low excitons diffusion length, between 10 and 20 nanometres. This means that in a bilayer junction, only excitons created within the diffusion distance of the interface contribute to the current flow. Excitons generated farther than diffusion length from an interface recombine before they have a chance to separate. The need to have a junction very close to the exciton generation sites, yet still have a device thick enough to absorb significant amounts of light, led to the development of another junction structure: the bulk heterojunction. In a bulk heterojunction, the same effect is used, but with nanoscale mixing of the donor and acceptor. Instead of having only a junction layer, there are junctions throughout the entire active layer. By placing a junction within the diffusion length of almost every exciton creation point, the efficiency of the device can be radically improved.



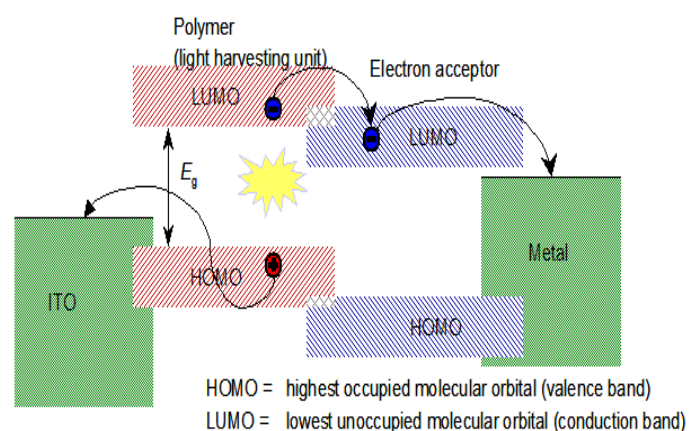
(Figure 5: Schematic diagram of a bulk heterojunction)

It is important to note that while a bulk heterojunction improves charge separation, it does it at the cost of increasing the distance and

complexity of the path that charges must travel. Furthermore, it places difficult morphological requirements on the active layer being as the donor and acceptor must not only be mixed on the nanoscale but also bicontinuous. It is our hope that replacing the donor with CNTs whose exciton diffusion length is greater than conductive polymers this strict morphological requirement can be relaxed without decreasing efficiency. The red represents the electron donor while the blue represents the electron acceptor.

3. Charge Separation

Charge separation occurs at a donor/acceptor junction when the local electric field generated by the difference in band gaps of the donor and the acceptor is large enough to overcome the Coulombic attraction of the excitons. The absorbance of a photon in the donor material promotes an electron to its LUMO, and leaves a hole in its HOMO. At the junction, the electron will jump from the donor's LUMO to the acceptor's LUMO because it is a lower energy state. The electrons will then travel "downhill" to the lower work function electrode, while the holes travel "uphill" to the high work-function electrode. Figure 6 illustrates this process.



(Figure 6: Band diagram of organic solar cell showing charge separation and transport)

4. Charge Transport

The final step for current generation is charge transport to their respective electrodes. Charge transport is guided by the electric field generated throughout the active layer by the difference in work functions of the electrodes. Band bending creates the "uphill" and "downhill" for the charges to travel. However, despite having a guiding electric field, charges can be lost as they travel to the electrode. Thus, it is important to minimize the distance and the complexity of the path that the

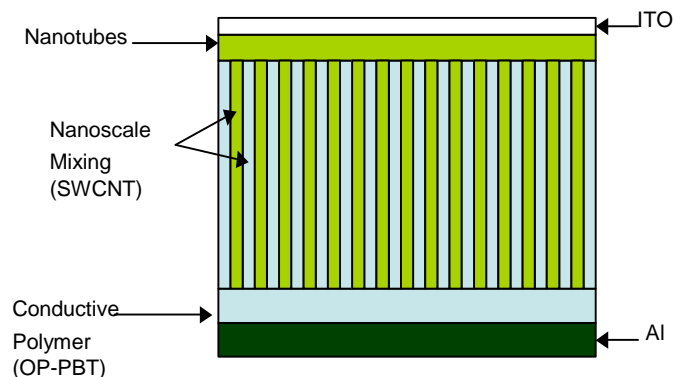
charges must travel. It is our hope that replacing the electron donor with CNTs which have a much better charge mobility, the amount of holes reaching the ITO electrode can be increased.

V. Efficiency of EOPV

With the application of Aluminium Studs the absorption of sunlight increases. And with the use of SWCNT and OP-PBT the interception bandwidth range of Solar Radiation Spectrum also increases. Infrared, Visible region and larger wavelengths are consumed. The reason behind this is, SWCNT utilises photons of larger wavelength and OP-PBT engulfs shorter wavelengths of the electromagnetic spectrum. As well as, SWCNT is a good electron donor and OP-PBT is a good electron acceptor. The current density of both the active materials are high which propels the generated electron hole pairs (from excitons) to their respective electrodes. This leads to a large quantity of photocurrent. Thus with the combination of all these materials the efficiency of solar cells will definitely increase and will surpass the existing solar cells efficiency.

VI. Conclusion

The design of these components came from background knowledge that we spent a considerable amount of time collecting previous literature on the topic of organic solar cells. It provided helpful information and directions for our project. This model is simply a theoretical proposal; there is still work to be done mathematically and experimentally to verify if even our basic modelling assumptions were accurate. An ideal EOPV structure is Checkerboard organic solar cell as it has orthogonal electric field. In this the excitons generated will quickly find the junction and pulled apart.



(Figure 7: An ideal EOPV structure)

But one of major challenge in the implementation of ideal EOPV is its fabrication. With the development in the fabrication and nanotechnology we can overcome this challenge. Our research team believes that this model has the potential that if further researches are continued in this project of EOPV (Enhanced Organic Photovoltaics) it will yield a better efficiency as well as it will be cost effective.

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