Optimizing the Design of Flexible PTB7:PC₇₁BM Bulk-Heterojunction and P3HT:SiNW Hybrid Organic Solar Cells

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Abstract

The design of flexible PTB7:PC₇₁BM bulk-heterojunction and P3HT:SiNW hybrid organic solar cells are optimized for maximum photovoltaic performance. The thickness of each layer is optimized for maximum photon absorption in the active layer of a bulk-heterojunction organic solar cell with structure, PET/PEDOT:PSS/TFB/PTB7:PC₇₁BM/Ca and that of a hybrid solar cell with structure, PET/PEDOT:PSS/TFB/P3HT:SiNW/Ca. The optimal design thus obtained produces a power conversion efficiency of 12.87% in the bulk-heterojunction and 4.70% in hybrid solar cell. High photon absorbance is found to occur within a wide range of the solar spectrum for PTB7:PC₇₁BM bulk-heterojunction organic solar cell while a high transmittance and reflectance is found in the P3HT:SiNW hybrid solar cell. This difference may be attributed to the wide band gap of P3HT and mismatch between the electron and hole mobilities in the hybrid solar cell. Nevertheless, the optimized design of the hybrid solar produces a power conversion efficiency greater than 50% measured experimentally.

Keywords: Organic solar cells; PTB7:PC₇₁BM bulk-Heterojunction; P3HT:SiNW Hybrid; Optimized design; Power conversion efficiency

Introduction

Research interest in organic solar cells (OSCs) has escalated drastically over the last decade due to their low-cost, flexibility, easy fabrication techniques and large-scale production [1-3]. However, low power conversion efficiencies (5-9.2%) [4-6] and stability [7] still limit their commercialization. The two most studied classes of OSCs are the bulk-heterojunction and hybrid types [8]. Former is the most efficient OSC known to-date with the donor and acceptor organic materials blended together forming an interface [9-11]. The concept of hybrid OSCs was developed with an intent of combining the advantages of both organic and inorganic materials, where the organic acceptor layer was replaced with an inorganic material for enhanced absorption and stability in the structure but maintaining the bulk-heterojunction concept [12,13].

The standard structure of an OSC comprises of a substrate, an anode, active layer (blend of donor and acceptor) and a cathode

[14]. In addition, a hole transport layer (HTL) and an electron transport layer (ETL) can be incorporated within the design as support layers [15-17]. The role of each of the layers in a multilayered structure is discussed below. The operation of an OSC depends primarily on the following four mechanisms:

- 1) Photon absorption leading to the creation of excitons [2,18],
- 2) Exciton diffusion to the donor-acceptor interface [1]
- 3) Exciton relaxation into a charge transfer exciton state and simultaneous dissociation into free charge carriers [3], and
- 4) Collection of holes at the anode and electrons at the cathode with the aid of the electric field created by the work function difference between the two electrodes [3].

In OSCs, the top-most layer is a substrate that provides support for growing the anode, for example, glass or transparent plastic. Glass is highly transparent over the visible spectrum, has advanced thermal properties such as high temperature stability and provides an excellent barrier against water and oxygen; however, it is very rigid [19]. On the other hand, plastic is highly flexible, inexpensive and compatible with roll-to-roll OSC fabrication but lack thermal stability. Common examples of plastic substrates include polyethylene terephthalate (PET), polyethylene naphthalate (PEN), polycarbonate (PC) and polyethersulfone (PES) [20-22]. For fabrication and modeling of flexible and lightweight OSCs, such as the ones used in this study, plastics are preferred over glass substrate.

The anode acts as a window for light penetration through to the active layer and provides the site for hole collection after exciton dissociation as mentioned in step 4 above. It must be highly transparent and conductive and common examples include indium tin oxide (ITO) [23] carbon nanotubes [24] graphene [25], poly(3,4-ethylenedioxythiophene) poly(styrenesulfonate) (PEDOT:PSS) [26,27] and zinc oxide (ZnO) [28]. ITO is the most popular choice because of its high electrical conductivity and optical transparency; however, it lacks flexibility due to high

mechanical brittleness [57] and is one of the expensive materials in the OSC design because indium is a very rare metal [19]. Cathode provides the site for electron collection after exciton dissociation and common examples include low work function metals such as Aluminium (Al), Calcium (Ca) and Silver (Ag) [30].

In the bulk-heterojunction and hybrid OSCs, the most important component is the active layer where majority of the processes take place [mechanisms (1)-(3)]. In bulk-heterojunction OSCs, the highest experimental power conversion efficiency (η) of 9.20% has been achieved through a combination of low-band gap semiconducting donor polymer, thieno [3,4-b]thiophene/benzodithiophene (PTB7) and a small molecule fullerene-derivative acceptor, [6,6]-phenyl C₇₁-butyric acid methyl ester (PC₇₁BM) [4]. In hybrid solar cells, a combination of silicon nanowires (SiNWs) and PEDOT:PSS have produced the best power conversion efficiency of 8.40% [31]. Furthermore, the HTLs facilitate hole transport between anode and active layer and ETLs help transport electron between the active layer and cathode. Examples of HTL include PEDOT:PSS [16], nickel oxide (NiO_x) [32], graphene oxide [33] and poly[9,9-dioctylfluorene-co-N-[4-(3-methylpropyl)]-diphenylamine] (TFB) [34] and those of ETLs include lithium fluoride (LiF) [15,35] titanium dioxide (TiO₂) and ZnO [17].

OSCs are considered to be optically active devices [36], which means more the absorption, better the performance. For efficient absorption of photons (mechanism 1), the absorption spectrum of the active layer must match with the solar spectrum. Also, the thickness of each layer within the design should be optimum to allow maximum absorption of photons in the active layer. However, upon illumination, the light is not only absorbed in a solar cell but is also reflected and transmitted at each layer [37]. The aim of this work is to optimize the design of OSCs using the semiconducting thin film optics simulation software (SETFOS), to achieve minimal reflectance and transmittance and optimal absorbance and power conversion efficiencies in the bulk-heterojunction and hybrid OSCs.

Optimization using SETFOS

Semiconducting thin film optics simulation (SETFOS) is an optical and electrical simulation software developed to simulate novel optoelectronic thin-film based solar cells [38]. Within the absorption and drift diffusion setting of SETFOS, the wavelength region is set in the range of 380-780 nm and the illumination to AM 1.5 with 1 sun. Transfer matrix approach is used in SETFOS to calculate the optical properties of a multilayer structure [36] and the absorption profile is derived by considering the complex refractive index, $N=n+ik$, of each layer, where n is the refractive index and k is the extinction coefficient [36]. The absorbance, A , of the multilayer structured cell is calculated from the conservation of energy as [38].

$$A+R+T=1 \quad (1)$$

Where R = reflection and T = transmission. The photon generation rate profile, $G(z)$, is given by:

$$G(z)=\int_{\lambda} \frac{\alpha(\lambda)I_{AM1.5}(z,\lambda)}{h\nu} d\lambda \quad (2)$$

Where $\alpha(\lambda)$ is the absorption coefficient at wavelength, λ , $I_{AM1.5}$ is the illumination irradiance at AM 1.5, $h\nu$ is the incident solar photon energy and z is the vertical position inside the device measured from the top layer as shown in Figure 1. Detailed methods and analysis used in SETFOS can be found in the work done by Fluxim [38]. For simulation in SETFOS, input parameters required are n and k values, layer thickness, energies of the highest occupied molecular orbital (HOMO), lowest unoccupied molecular orbital (LUMO), electron and hole mobilities and dielectric constant etc., for each layer incorporated within the multilayer design.

Incorporating the input parameters in SETFOS, the thickness of each layer is optimized for maximum photon absorption in the active layer. The spectral, optical and electrical profiles are generated and their key current-voltage (I-V) characteristics are obtained by SETFOS. After optimizing the structure, SETFOS calculates the power conversion efficiency, η of the solar cells using [14].

$$\eta=\frac{V_{oc}J_{sc}FF}{P_{in}} \quad (3)$$

Where V_{oc} = open circuit voltage, J_{sc} = short-circuit current

density, P_{in} = input power (100 m W cm⁻²) and $FF=\frac{V_m J_m}{J_{sc} V_{oc}}$

is the fill factor with V_m = maximum voltage and J_m = maximum current density. Here SETFOS is used to optimize the simulation of two kinds of OSCs:

1. PTB7:PC₇₁BM bulk-heterojunction and

Figure 1: Schematic layer design of an organic solar cell as a function of the vertical position, z , inside the device measured from the top layer as used in SETFOS.

2. P3HT:SiNW hybrid solar cells.

Optimization of PTB7:PC₇₁BM bulk-heterojunction OSC

For modelling the bulk-heterojunction OSCs, PTB7 and PC₇₁BM are chosen as the donor and acceptor organic materials, respectively, because of their more desirable optoelectronic properties leading to a higher conversion efficiency [4,39]. PET is chosen as the substrate and PEDOT:PSS as the anode. TFB and Ca are chosen as the HTL and cathode, respectively, in the flexible ITO-free PTB7:PC₇₁BM bulk-heterojunction OSC. The following input data are used in the optimization of the design of a bulk-heterojunction OSC. The work function (Φ) of the electrodes are: PEDOT:PSS = -5 eV [26] and Φ_{Ca} = -2.9 eV [19] and their optical data (n and k values) are obtained from the work done by Palik and Ghosh [40]. For TFB, $LUMO$ = -2.3 eV, $HOMO$ = -5.3 eV and μ_h = 5×10^{-4} cm²V⁻¹s⁻¹ [34]. For PTB7:PC₇₁BM active layer, $LUMO_{PTB7}$ = -3.31 eV, $HOMO_{PTB7}$ = -5.15 eV, $LUMO_{PC_{71}BM}$ = -4.30 eV and $HOMO_{PC_{71}BM}$ = -6.10 eV [39], dielectric constant (ϵ) = 3.9, ϵ_e = 4.4×10^{-4} cm²V⁻¹s⁻¹ and μ_h = 5.8×10^{-4} cm²V⁻¹s⁻¹ [41]. The n and k values of PTB7:PC₇₁BM are obtained from the work of Zhicai et al. [4]. The structure of the bulk-heterojunction OSC used in the optimization by SETFOS is: PET/PEDOT:PSS/TFB/PTB7:PC₇₁BM/Ca.

Optimization of P3HT:SiNW hybrid OSC

For the simulation of hybrid OSCs, P3HT (polythiophene) and silicon nanowires (SiNWs) are chosen as the organic donor and inorganic acceptor, respectively [42]. P3HT is a wide band gap polymer and is the most popular and studied donor material used in organic photovoltaics [43,9] and SiNWs ensure large donor-acceptor interfacial area with continuous interpenetrating pathways for better charge transport to the electrodes [44]. In this simulation, PET is chosen as the substrate, PEDOT:PSS as the anode, TFB as the HTL and Ca as the cathode, forming flexible ITO-free P3HT:SiNW hybrid OSC. For the P3HT:SiNW active layer, n and k values [45,46] are generated using the effective medium approximation within SETFOS with $LUMO_{P3HT}$ = -3.20 eV, $HOMO_{P3HT}$ = -5.2 eV [29], μ_h = 2×10^{-3} cm²V⁻¹s⁻¹ [36], conduction band energy, CB_{SiNW} = -4.0 eV, valence band energy, VB_{SiNW} = -5.10 eV [47] and μ_e = 350 cm²V⁻¹s⁻¹ [48]. The optical and electrical data for the other layers are the same as for the PTB7:PC₇₁BM bulk-heterojunction OSC described in section 2.1. The structure of the hybrid OSC used in the optimization by SETFOS is: PET/PEDOT:PSS/TFB/P3HT:SiNW/Ca.

Results and Discussion

In this section, the optimized structures of PET/PEDOT:PSS/TFB/PTB7:PC₇₁BM/Ca and PET/PEDOT:PSS/TFB/P3HT:SiNW/Ca and their optical, spectral and electrical profiles are presented. In both the optimizations, the thickness of the substrate, PET, is fixed at 1000 nm [49].

Results of optimization of PTB7:PC₇₁BM bulk-heterojunction OSC

Having chosen the anode, HTL, active layer and cathode, the thickness of each of the layers is optimized for maximum photon

absorption in the active layer. The thickness of each layer in the optimal design is obtained as given in Table 1.

The reflectance, transmittance and absorbance [calculated from Eq. (1)] and photon generation rate [calculated from Eq. (2)] for the optimal structure of PET/PEDOT:PSS/TFB/PTB7:PC₇₁BM/Ca bulk-heterojunction OSC is shown in Figure 2: (a) reflectance (b) transmittance (c) absorbance and (d) the photon generation rate.

According to Figure 2 (a)-(c), the absorbance in the optimized structure of an OSC is found to be very high ~ 0.90 (90%) within a spectrum range 380-650 nm, after which it declines due to high transmittance and reflectance as obtained from the conservation Eq. (1). Reflectance is greater than transmittance in the higher wavelength region. In order to reduce the reflection, a possible solution would be to employ a layer of anti-reflection coating on PET. The highest absorbance is found to occur in the PTB7:PC₇₁BM layer, followed by that in Ca, with only a negligible absorbance appearing to occur in PEDOT:PSS and TFB. The absorbance in the whole OSC structure occurs mostly in the active layer, as it can be seen from Figure 2(c). Also, the photon generation rate gets intensified in the active layer as shown in Figure 2(d) with a maximum rate of 1.7×10^{19} m⁻²nm⁻¹s⁻¹ at z = 1050 nm layer position in the optimized structure. Overall, the combination of PTB7 and PC₇₁BM as the active layer is found to be very effective as it provides a broad range absorption of the solar spectrum.

The current-voltage (I-V) characteristics of the optimized PET/PEDOT:PSS/TFB/PTB7:PC₇₁BM/Ca bulk-heterojunction OSC is shown in Figure 3. The measured values of V_{oc} , J_{sc} , V_m , J_m , FF and η [Eq. (3)] obtained from Figure 3 are listed in Table 2.

According to Table 2. The optimized structure produces a conversion efficiency of 12.87%, which is 56.19% higher than the measured efficiency to-date of 9.2% [4]. This enhancement in the conversion efficiency can be attributed to the optimized design of the PET/PEDOT:PSS/TFB/PTB7:PC₇₁BM/Ca bulk-heterojunction OSC simulated by SETFOS.

Results of optimization of P3HT:SiNW hybrid OSC

For the hybrid structure, the thicknesses of the anode, HTL, active layer and cathode are optimized for maximum photon absorption in the active layer. The thicknesses in the optimal structure thus obtained are given in Table 3.

Layer	PEDOT:PSS	TFB	PTB7:PC ₇₁ BM	Ca
Thickness (nm)	25	1	69	100

Table 1: Thicknesses of each layer in the optimal design of a PTB7:PC₇₁BM bulk-heterojunction OSC.

Parameter	V_{oc} (V)	J_{sc} (mA cm ⁻²)	V_m (V)	J_m (mA cm ⁻²)	FF	η (%)
Value	1.32	-13.61	1.10	-11.7	0.72	12.87

Table 2: I-V parameters obtained from the optimized structure of PET/PEDOT:PSS/TFB/PTB7:PC₇₁BM/Ca OSC.

Figure 2: Plots of (a) Reflectance (b) Transmittance and (c) Absorbance as a function of the solar spectrum wavelength and (d) Photon generation rate as a function of the layer position, [Eq. (2)] in the optimized structure of a PET/PEDOT:PSS/TFB/PTB7:PC71BM/Ca bulk-heterojunction OSC.

The reflectance, transmittance and absorbance [calculated from Eq. (1)] and photon generation rate [calculated from Eq. (2)] for the optimal structure of PET/PEDOT:PSS/TFB/ P3HT:SiNW/ Ca hybrid solar cell is shown in Figure 4: (a) reflectance (b) transmittance (c) absorbance and (d) the photon generation rate.

In the optimized structure of PET/PEDOT:PSS/TFB/ P3HT:SiNW/ Ca hybrid OSC, the reflectance and transmittance are found to increase drastically at wavelengths higher than 500 nm of the solar spectrum and as a result, low absorbance is obtained from the whole structure in this region as shown in Figure 3 (a)-

Layer	PEDOT:PSS	TFB	P3HT:SiNW	Ca
Thickness (nm)	25	1	100	100

Table 3: Optimized thickness of each layer in the P3HT:SiNW hybrid OSC.

(c). The highest absorbance is found to occur in the P3HT:SiNW active layer, followed by that in Ca cathode. PEDOT:PSS and TFB both show negligible absorbance. Overall, the highest absorbance of 0.84 (84%) occurs at a wavelength of 490 nm and the maximum photon generation rate of $1.05 \times 10^{19} \text{ m}^{-2} \text{ nm}^{-1} \text{ s}^{-1}$ occurs at $z = 1075 \text{ nm}$ in the optimized structure as shown in Figure 3(d). The combination of P3HT:SiNW as the active layer thus provides an absorption in the narrower region of the solar spectrum as compared to the PTB7:PC₇₁BM bulk-hetero junction OSC.

The current-voltage (I-V) characteristics of the optimized PET/PEDOT:PSS/TFB/P3HT:SiNW/Ca hybrid OSC is shown in Figure 5 and the values of V_{oc} , J_{sc} , V_m , J_m , FF and η [(Eq. (3))] are listed in Table 4.

Figure 3: I-V curve of the optimized PET/PEDOT:PSS/TFB/PTB7:PC71BM/Ca OSC.

According to Table 4, the conversion efficiency from the optimized structure is found to be 4.70%, which is 143.52% higher than the measured conversion efficiency to-date of 1.93% [42]. This enhancement in the conversion efficiency may be attributed to the optimized design of the PET/PEDOT:PSS/TFB/P3HT:SiNW/Ca hybrid solar cell simulated by SETFOS. However, the optimal conversion efficiency of the hybrid is only half of that obtained from the optimal PTB7:PC₇₁BM bulk-heterojunction OSC.

Comparative Performance of optimized PTB7:PC₇₁BM bulk-hetero junction and P3HT:SiNW hybrid OSCs

In the above optimal designs, the HTL is found to be the thinnest layer in the overall structure and the active layers are obtained to be 69 nm for PTB7:PC₇₁BM bulk-heterojunction and 100 nm for P3HT:SiNW hybrid OSC as shown in Table 1 and 3, respectively. Comparing Figures 2 & 4, PTB7:PC₇₁BM bulk-heterojunction OSC shows a higher absorbance and photon generation rate compared to P3HT:SiNW hybrid OSC. This can be attributed to the lower band gap of PTB7 (1.84 eV) [39] than P3HT (2 eV) [29], which allows more photon absorption from a broader range of the solar spectrum [50].

According to the dissociation mechanism outlined in our previous work [3], after the photon absorption and Frenkel exciton formation, the exciton diffuses to the interface and relaxes to a charge transfer (CT) exciton state by releasing the excess energy to molecular vibrations (phonons). If this excess vibrational energy released impacts back to the CT exciton, it can dissociate into free charge carriers. In PTB7:PC₇₁BM bulk-heterojunction OSC, this vibrational energy is provided by the LUMO offset between the PTB7 and PC₇₁BM. Likewise in P3HT:SiNW hybrid OSC, the vibrational energy is generated from the offset between the LUMO of P3HT and conduction

band of SiNWs. In PET/PEDOT:PSS/TFB/PTB7:PC₇₁BM/Ca bulk-heterojunction OSC, the vibrational energy is 0.99 eV and in PET/PEDOT:PSS/TFB/P3HT:SiNW/Ca hybrid OSC, it is 0.80 eV. This much excess vibrational energy is adequate to dissociate both singlet and triplet excitons in both heterojunction and hybrid OSCs. Also, at such a large available excess energy, the dissociation of an exciton may be faster than the non-radiative recombination, which enhances the performance of an OSC [18,3]. The dissociated free electrons and holes are collected by the work function difference between the electrodes i.e. $\Phi_{\text{PEDOT:PSS}} - \Phi_{\text{Ca}} = 2.10$ eV, which creates a reasonably large built-in field for efficient transport and collection of holes at PEDOT:PSS and electrons at Ca, in both OSCs.

The power conversion efficiency is dependent on the photon absorption efficiency (η_{abs}), exciton diffusion efficiency (η_{dif}), exciton dissociation efficiency (η_{dis}), and free charge carrier collection efficiency (η_{cc}) [51]. The external quantum efficiency (η_{ext}) of an OSC is then given as [52,58].

$$\eta_{\text{ext}} = \eta_{\text{abs}} \eta_{\text{dif}} \eta_{\text{dis}} \eta_{\text{cc}} \quad (4)$$

In the optimal design obtained here for both the OSCs, η_{dif} and η_{dis} have increased because of the bulk-heterojunction concept of the OSCs and the sufficient available excess vibrational energy at the donor-acceptor interface to overcome the exciton binding energy [1,3]. According to Table 2 and 4, the power conversion efficiency of the PTB7:PC₇₁BM bulk-heterojunction OSC is about three times larger than that of P3HT:SiNW hybrid OSC. This may be attributed to the fact that η_{abs} and η_{cc} are higher in PTB7:PC₇₁BM bulk-heterojunction OSC than in P3HT:SiNW hybrid OSC. The lower band gap of PTB7 leads to a high photon absorption efficiency in PTB7:PC₇₁BM bulk-heterojunction. On the other hand, in P3HT:SiNW hybrid OSC, the wide band gap of P3HT reduces η_{abs} because in the lower energy range, photons cannot be absorbed [53]. This affects the J_{sc} of each device [54] as can be seen from Table 2 and 4, where the absolute value of J_{sc} in P3HT:SiNW hybrid is 1.6 times smaller than that of PTB7:PC₇₁BM bulk-heterojunction OSC.

Also, considering the charge transport in P3HT:SiNW hybrid OSC, the electron mobility is much higher than the hole mobility, $\mu_e > \mu_h$ i.e. electron will reach the Ca electrode much faster than the hole can reach PEDOT:PSS. This leads to hole accumulation within the bulk which may lead to non-radiative quenching of holes and a low free carrier collection efficiency. On the other hand, for PTB7:PC₇₁BM bulk-heterojunction OSC, the electron and hole mobilities are nearly the same, which leads to high free charge carrier collection efficiency. Charge transport affects the fill factor of the device [54] as shown in Table 2 and 4 i.e. the *FF* of P3HT:SiNW hybrid is 1.5 times less than that of PTB7:PC₇₁BM bulk-heterojunction OSC. The V_{oc} of both types of OSCs is dependent on the energy levels between the donor and acceptor and the built-in potential due to their work function difference (2.10 eV) [55,56], which are higher in these optimized OSCs. Hence, our designs for both types of OSCs can be expected to help in the fabrication of more efficient bulk-heterojunction and hybrid solar cells.

Figure 4: Plots of (a) Reflectance (b) Transmittance and (c) Absorbance as a function of the solar spectrum wavelength and (d) Photon generation rate as a function of the layer position, [Eq. (2)] in the optimized PET/PEDOT:PSS/TFB/P3HT:SiNW/Ca hybrid OSC.

Parameter	V_{oc} (V)	J_{sc} (mA cm ⁻²)	V_m (V)	J_m (mA cm ⁻²)	FF	η (%)
Value	1.22	-8.03	0.90	-5.22	0.48	4.70

Table 4: I-V parameters obtained from the optimized structure of PET/PEDOT:PSS/TFB/ P3HT:SiNW/Ca OSC.

Conclusions

The design of PET/PEDOT:PSS/TFB/PTB7:PC₇₁BM/Ca bulk-heterojunction and PET/PEDOT:PSS/TFB/P3HT:SiNW/Ca hybrid OSCs has successfully been optimized using SETFOS. The thickness of the layers within each structure is optimized with respect to the maximum photon absorption in their active layers. High conversion efficiencies of 12.87% and 4.70% are obtained for PTB7:PC₇₁BM bulk-heterojunction and P3HT:SiNW hybrid OSCs, respectively. PTB7:PC₇₁BM absorbs a broad region

of the solar spectrum due to its low band gap. The offset at the donor and acceptor interface also generates adequate vibrational energy to dissociate both singlet and triplet excitons and the large built-in field between PEDOT:PSS and Ca work functions facilitate the transport and collection of free charge carriers in both OSCs. However, the wide band gap of P3HT and the unbalanced electron and hole mobilities affect the performance of the optimized P3HT:SiNW hybrid OSC. Overall, after the design optimization of both PTB7:PC₇₁BM bulk-heterojunction and P3HT:SiNW hybrid OSCs, a higher power conversion efficiency is

Figure 5: I-V curve of the optimized PET/PEDOT:PSS/TFB/P3HT:SiNW/Ca OSC.

obtained in both types of OSCs. It is expected that these optimal designs will help in the fabrication of higher efficiency OSCs.

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