A new approach of using area under the curve of absorption profile to optimize the active layers of photovoltaic devices

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Research Article

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Abstract

Optimization of photovoltaic (PV) active layers is usually carried out in terms of the energy bandgap ($E_g$) variation of the bulk heterojunction (BHJ) layers. However, the non-monotonic change in the $E_g$ does not guarantee the achievement of a maximum absorption capability at the optimum condition despite the broadened absorption spectrum. Hence, alternative strategies need to be researched in order to assign the best possible condition at which the active layer can convert the highest possible number of exposed photons to free electrons when it is employed in PV devices. Therefore, in this work, we propose a new approach which can be effectively used to optimize the BHJ active layers in terms of photon to electron conversion, considering the absorption profile of the system. Herein, area under the curve (AUC) of the absorption profile is utilized to optimize the active layers of photovoltaic devices. To formulate the proposed technique, a ternary system based on P(TRI-co-TER):Beetroot dye:PINDOLE was investigated and analyzed. Results showed that a linear correlation was produced between the AUC and photocurrent density ($J_{ph}$), which can be ultimately used to optimize the active layers of PV devices.

1. Introduction

In the last decades, the electronic industry experienced a pronounced development, focusing on the organic and inorganic based devices such as sensors, organic light emitting diode (OLED), and solar cells [1–6]. Because of the high cost and high energy demand in the fabrication process of inorganic based devices, organic materials have received a considerable attention to be utilized in electronic devices [7–12]. Therefore, several approaches have been employed to improve the performance of organic based devices, including device architecture, active layer optimization and the use of different fabrication techniques [11–16]. More specifically, the structure and type of active layer materials have a critical impact on the device performance [17, 18]. Thus, selecting the raw materials and their ratio has an ultimate effect on the device performance. Charge carriers’ generation in the conjugated polymers due to the absorption of electromagnet waves are distinct from that in the inorganic materials. In the inorganic materials, free holes and electrons are directly generated upon photon absorption, while in organic materials excitons are initially formed, requiring some additional energy to dissociate them into free holes and electrons. Subsequently, the formation of free carriers in a single layer of organic photovoltaic device is too low, yielding a low efficiency device [19]. One of the obstacles to dissociate excitons is the inherent excitons binding energy which is more than the thermal energy. Besides, the short diffusion length of excitons is another factor hinders efficient generation of free holes and electrons at the offset energy boundaries between the electron donor and acceptor moieties. Therefore, a built-in potential of around 0.3V is required for the dissociation which is formed from the differences of LUMO levels between acceptor and donor conjugated polymers. Thus, bulk heterojunction (BHJ) structure, which comprises of blending donor and accepter materials, was proposed to overcome the problems of bilayer structures [20, 21]. On the other hand, to broaden the absorption spectrum and improve charge generation in the organic active layers, ternary bulk heterojunction (TBHJ) structure was proposed. Several strategies have been
employed for selecting the third component in the ternary systems in terms of different energy gaps or similarity in molecular structure [22–24].

The process of enhancing photon absorption by the active layers is very important to achieve a better solar cell device performance. This is because the increased photon absorption is directly related to the increased amount of generated charge carriers, thereby increasing the photo current of the device [25–27]. An extensive review of literature showed that red shifting (increased wavelength) in the absorption spectrum of the active layers was mainly considered to optimize the materials to be selected for efficient photo-absorption and device performance. However, it is well known that the overall broadening of the absorption spectrum in the entire wavelength region is crucial for the increased amount of photo-generated current. That means not only the low energy gap of the active layer, which is interpreted by its red shifted absorption spectrum, is responsible for the increased photon absorption, but the number of photons that are capable to be captured by the active layer is also playing a crucial role in defining the external quantum efficiency of the photovoltaic devices [28]. Therefore, we anticipate that estimating the area under the curve of the optical absorption profile of the materials can be another useful approach to be used to optimize the active layers of photovoltaic devices. Up to now, UV-visible spectroscopy, which is an analytical tool, is used for both qualitative and quantitative measurements. In the pharmaceutical and biological field, the UV-Vis spectrum was also used to measure the concentration of the components and protein detection [29–31]. In addition, the derivation and integration of the absorption spectrum were used for analysing drug components and their concentrations [32–35]. Therefore, in this work electron-rich donor; Poly [triamterene-co-terephthalate] (P(TRI-co-TER)), and one electron-deficient acceptor, Poly (5-hydroxyindole-2-carboxylate)(PINDOLE) are blended with natural dyes from beetroot in order to produce ternary systems representing a representative active layer. Consequently, the absorption spectra of the active layer are recorded and used to build our proposed approach, which is based on evaluating the ratio and concentration of the ternary active medium. The absorption profile is built based on the measured absorption spectrum of the material and the global irradiance, as it is explained in details in the methodology section.

2. Materials And Method

In this work, a ternary composite system was chosen as a representative active layer of photovoltaic devices. The active layer is made of the combination of donor, acceptor and dye materials. The absorption profile of the active layer was therefore deduced to validate the concept of using area under the curve (AUC) of the absorption profile to optimize the active layer for the best performance of solar cells in terms of photo-generated current density ($J_{ph}$), which is an essential photovoltaic parameter defining the performance of the device. It is known from literature that the value of $J_{ph}$ can be determined by using the following equation [36, 37]:

$$J_{ph} = \frac{q}{hc} \int A(\lambda)AM1.5G(\lambda) \lambda d\lambda$$

(1)
where $h$ is the Plank’s constant, $A$ is the solar cell area, $c$ is the speed of light and $A.M1.5G$ is the spectral irradiance of the light, as shown in Fig. 1 [38]. Therefore, in this proposed approach, we have defined the absorption profile by the integral part of Eq. 1.

The utilized donor, acceptor and dye (beetroot extracted dye) materials were synthesized following the methods described in our previous works [39, 40]. UV–Vis spectrophotometer (UV line 9400) were used to measure the optical absorption spectra of the investigated samples at room temperature. The samples were prepared by blending the donor and acceptor with the natural dye, which are denoted by [P(TRI-co-TER): Beetroot dye: PINDOLE] throughout the manuscript. Hence, the ratio of the acceptor and natural dye was changed separately with respect to the donor component. Consequently, the ratio of both donor and acceptor was fixed at (1:1) and the natural dye was added to the binary system. As such, the absorbance spectrum for each ternary system was measured from 200 nm to 800 nm. Later on, area under the curve (AUC) for each absorption profile of the measured samples was calculated by using Eq. 1. Subsequently, the photogenerated current density ($J_{ph}$) was determined considering the absorption profile of the samples in the wavelength range 280 nm to 650 nm. In this way, the presence of a direct relation between the photogenerated current and area under the curve (AUC) of the absorption profile can be interestingly interpreted to assign the optimum content of the dye in the ternary active layer. Similarly, by fixing the dye ratio, it is possible to find the optimal ratio of the accepter component following the same procedures that was previously employed for finding the optimum ratio of the dye. Consequently, the concept of area under the curve of absorption profile can be successfully utilized to optimize the acceptor and natural dye contents within the ternary system.

3. Results And Discussion

In general, four processes are occurred within the active layer of photovoltaic devices upon the absorption of photon energy, including (a) exciton generation due to the photon harvesting, (b) diffusion of excitons toward the donor-acceptor interface, (c) generation of free charge carriers because of exciton dissociation, and (d) transport of charge carriers and charge collection by the respective electrodes [41]. Each step has a crucial impact on the device performance, and the most essential photovoltaic parameter defining the solar cells efficiency is the photocurrent density ($J_{ph}$), which is described in terms of photon to free electronic charge conversion. Therefore, due to the absorption of photons at the donor-acceptor interface, intramolecular singlet excitons are generated as a result of charge transfer (CT) in the active medium, thereby moving the free electrons and holes toward their respective electrodes [36, 42]. As such, four possible transport models for ternary organic solar cells were reported in literature, namely charge transfer, energy transfer, parallel-linkage, and alloy model [43–45]. To this end, the spectral studies might reveal further significant information on the photocurrent density ($J_{ph}$) and it is related to the incident photon flux $G(\lambda)$ and absorption spectrum $A(\lambda)$, which is a wavelength dependent function and is defined by the number of charges leaving the electrodes per second with respect to the incident optical power for the solar spectrum (see Eq. 1).
Alternatively, in the device efficiency, both irradiance and cell area can be taken into account according to Eq. 2 [28]:

\[ \eta = \frac{P_{out}}{P_{in}} = \frac{FF \times V_{oc} \times I_{sc}}{S \times A} \]  

where \( FF \) is the fill factor, \( V_{oc} \) is open circuit voltage, and \( I_{sc} \) is the short circuit current. In this context, the efficiency of the photovoltaic device is directly proportional to the incident optical power and the photocurrent. Figure 2(a) shows the absorbance spectra of the ternary system when the dye ratios have been changed. Consequently, one can assess the photogenerated current from absorbance spectra and spectral irradiance using Eq. 1, thereby integrating the absorption profile, as depicted in Fig. 2(b) in the wavelength range from 280 to 650 nm, which is the active absorption range of interest for our investigated samples. Herein, a linear relation perceived between the estimated photogenerated current and area under the curve of the absorption spectra with the change of the dye ratio, as can be seen in Fig. 3. A substantial change in the absorbance spectra was observed at the low ratio of beetroot when it was blended with P(TRI-co-TER):PINDOLE, while at the upper volume ratio, the spectrum was slightly changed. Thus, it can be difficult to select a broad spectrum which covers as the highest possible range of wavelength at the given dye ratio. Therefore, finding AUC by the integration of absorption profile can be a very good approach to find the best ratio of the dye. Noteworthy, the occurrence of a linear relation between the AUC and \( J_{ph} \) validates our proposed approach, by which the active layer can be optimized from the estimated AUC.

To estimate the optimal acceptor ratio for the ternary system, the content of the natural dye was fixed at the optimum value then the acceptor ratio was changed and the absorbance data were measured, as shown in Fig. 4(a). Nevertheless, no significant change was observed for the absorbance and absorption profile spectra (Fig. 4(b)) so that they can be directly used to choose the optimum value of the acceptor ratio. Alternatively, area under the curve (AUC) of the absorption profile was calculated at each acceptor content, as shown in Fig. 5. Consequently, the optimum content of the acceptor, at which the system is capable of providing the highest \( J_{ph} \), was assigned to be 2.05, while for the all three components are given in Table 1.

<table>
<thead>
<tr>
<th>Ternary System</th>
<th>Donor ratio</th>
<th>Dye ratio</th>
<th>Acceptor ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>P(TRI-co-TER): Beetroot: PINDOLE</td>
<td>1</td>
<td>1.9</td>
<td>2.05</td>
</tr>
</tbody>
</table>

4. Conclusions

In this work, a new approach was successfully proposed to optimize the BHJ active layers of photovoltaic devices, taking into account area under the curve (AUC) of their absorption profile. The best performance
of solar cells in terms of photo-generated current density \( (J_{ph}) \) could be defined through optimizing the absorption profile of the active layer. Results showed that a linear correlation can be produced between the AUC and photocurrent density \( (J_{ph}) \), which can be ultimately used to optimize the active layers of the PV devices.

**Declarations**

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**Conflicts of interest**

The authors declare that there is no conflict of interest regarding the publication of this paper.

**Author contributions**

Methodology: Peshawa O. Amin; Conceptualization: Fahmi F. Muhammadsharif; Writing - original draft preparation: Peshawa O. Amin; Writing-review and editing: Fahmi F. Muhammadsharif, Salah Raza Saeed, Kamal Aziz Ketuly; Formal analysis and investigation: Fahmi F. Muhammadsharif, Salah Raza Saeed, Kamal Aziz Ketuly; Supervision: Fahmi F. Muhammadsharif, Salah Raza Saeed.

**Availability of data and material**

The data and material are available within the manuscript.

**References**


25. Muhammadsharif, F.F., A new simplified method for efficient extraction of solar cells and modules parameters from datasheet information.: 2021


**Figures**
Figure 1

Spectral irradiance of the Sun (AM1.5 Global spectrum).

Figure 2

Absorbance spectra (a), and absorption profile versus wavelength (b) for the ternary P(TRI-co-TER): PINOLE: Beetroot dye system.
Figure 3

Plot of area under the curve (AUC) versus photogenerated current for the ternary P(TRI-co-TER): PINDOLE: Beetroot dye system.
Figure 4
Absorbance spectra (a), and (b) absorption profile versus wavelength for the ternary Beetroot dye:P(TRI-co-TER):PINOLE system.

Figure 5
Plot of absorption profile versus acceptor volume ratio for ternary Beetroot dye: P(TRI-co-TER): PINOLE