Effect of D-π-A indoline light absorbing layer on the performance of all organic photovoltaic devices.

Elyes Jbira and Hassen Derouiche

EasyChair preprints are intended for rapid dissemination of research results and are integrated with the rest of EasyChair.

October 11, 2019
Effect of D-π-A indoline light absorbing layer on the performance of all organic photovoltaic devices

Elyes Jbira
Laboratory of Smart Grid and Nanotechnology
National School of Sciences and Advanced Technologies of Borj Cédria
Technopole of Borj-Cédria Hammam-Lif, Tunisia
elyes_jbira@yahoo.com

Hassen Derouiche
Laboratory of Smart Grid and Nanotechnology
National School of Sciences and Advanced Technologies of Borj Cédria
Technopole of Borj-Cédria Hammam-Lif, Tunisia
hassen.derouiche@ensta-b.ru.tn

Abstract—In order to enhance the photovoltaic performance of all organic solar cells, a novel design is demonstrated by introducing a light absorbing layer of D149 indoline dyes in the P3HT:PCBM organic solar cells. The effect of D149 layer on the performance of the solar cells was explored by current-voltage (I-V) measurements. It was found that the maximum power conversion efficiency of the solar cells containing D149 light absorbing layer reached 4.51 %, which is much higher than that containing only P3HT:PCBM as the active layer (3.24%). The improvement finds its origin in a higher number of created electrons at photo-active layer/cathode interface via reinforcement of the light-absorbing property of the organic photovoltaic devices.

Keywords—All organic photovoltaic devices; BCP; D149 indoline dyes; D-π-A dyes; P3HT; fullerenes

I. INTRODUCTION

All organic photovoltaic devices are becoming increasingly efficient due to the discovery of new photo sensible molecules. Recently, a series of Donor-π-Acceptor (D-π-A) photosensitive dyes have been synthesized, with the donor and acceptor linked by a molecular bridge conductor (π-group) [1]. Under illumination, electrons in the HOMOs, situated around the donor group, are excited into the LUMOs, which are situated around the acceptor. This excitation process increases both the intramolecular charge transfer (ICT) and the photo generation of the electron [2, 3]. The metal-free indoline dye D149 is one of the most promising candidates for highly efficient and long-term stable All organic photovoltaic devices because of the high absorption of visible radiation and is able to improve the interface between the organic active layer and the cathode [4]. D149 Donor-π-Acceptor (D-π-A) with indoline as electron donor and a rhodanine as electron acceptor shows high photon-to-current efficiency and high molar absorption coefficients [5, 6].

Bulk heterojunction structures use a traditional active layer consisting of a blend of organic electron donor and acceptor components; while the donor component is a photosensitive conjugated polymer, the acceptor component is a fullerene derivative [7]. In order to achieve high performance all-small-molecule organic solar cells, the conjugated polymer must collect a wide range of visible light and possess good hole mobility. The transfer of charges can be made possible at the interface between these D/A materials providing that the conjugated polymer has the HOMO and LUMO levels lower than the fullerene derivative. The power conversion efficiency (PCE) of organic photovoltaic devices has already exceeded 9 % [8]. For the active layer, P3HT:PCBM bulk heterojunction composite was used; thus, this structural architecture increases the number of donor/acceptor interfaces and reduces the dissociation of excitons, resulting in a highly efficient active layer. D149 light absorbing layer was deposited on top of P3HT:PCBM to absorb the photons which were not absorbed by the active layer, therefore increasing the photocurrent of the all-small-molecule organic solar cells. To achieve the organic solar cells, Bathocuproine (BCP) has been used as hole-blocking layer [9]. BCP has a deep level of HOMO (7 eV), and a LUMO level (3 eV) substantially higher than the work function of aluminum (4.2 eV), which will block the diffusion of holes from the P3HT:PCBM/D149 layer to the cathode.

In this work, we have investigated the structural, optical and electrical properties of P3HT:PCBM organic photovoltaic devices and we also have studied the role played by a second absorbing layer of D149 indoline dyes on the photovoltaic characteristics.

II. EXPERIMENTAL METHODS

ITO-coated glass substrates were treated with a H2O-H2O2 (30%-NH4OH (25%) solution (5:1:1 vol parts) for 15 min, followed by rinsing with distilled H2O for 10 min in an ultrasonic bath. PEDOT:PSS, is a hole transporting conductor, having a good charge transport properties (conductivity of 1 S/cm). PEDOT:PSS was purchased from Aldrich, in aqueous dispersion with H2O as pristine solvent and has been spin coated onto ITO coated glass substrates and heated at 120 °C for 2 h. P3HT (SigmaAldrich, regioregularity ~ 96%) and PCBM (SigmaAldrich, 99.5% purity) were dissolved into a dichlorobenzene solution at a weight ratio 1.2:1 in a controlled nitrogen atmosphere at the ambient temperature in a glove box. The mixtures were spin coated (450 rpm, 60 s) on top of the ITO/PEDOT:PSS layer. The thickness was checked by cross-section visualization using a scanning electron microscope (SEM). A solution made of 0.3 mM D149 indoline dye (SigmaAldrich) in an acetonitrile/tert-butyl alcohol mixture (v/v = 1: 1) was spin coated on top of the P3HT:PCBM layer and heated at 70 °C for 1 h. Finally, BCP and Al upper contacts were deposited using vacuum evaporation at a pressure of 10-5 Pa. After thermal evaporation, the devices were annealed at 120 °C for 30 min.
III. RESULTS AND DISCUSSION

The AFM morphology of P3HT: PCBM and D149/P3HT: PCBM thin films is shown in Figure 1. P3HT: PCBM bulk heterojunction film on top of ITO/ PEDOT:PSS films (Figure 1.a) appears as an uniform P3HT matrix blended with PCBM near-spherical shape molecules; the bulk heterojunctions improve exciton dissociation process in the active layer of the all-small-molecule organic solar cells. The structure and surface morphology of D149 on top of P3HT: PCBM thin films (Figure 1.b) were found to be uniform and homogeneous. The indoline dye decreases the surface roughness, which leads to efficient charge transfer and collection at the interface between the active layer and BCP/Al cathode.

Fig. 1. AFM image of: (a) P3HT: PCBM thin film and (b) P3HT: PCBM/D149 thin film.

Figure 2 presents the absorption spectra for P3HT: PCBM and D149 thin films. P3HT: PCBM thin film shows a sharp absorption maximum at 492, 560 and 610 nm corresponding to the absorption of P3HT and the large absorption band in the range of 300-550 nm, with a maximum at 335 nm, corresponding to the absorption of PCBM [10]. For D149 thin film, the absorption spectrum exhibits two broad peaks in the range of 335-380 nm and 450-510 nm; the low energy peak (450-510 nm) is attributed to intramolecular charge transfer (ICT) from the indole donor to the acceptor, whereas the peak corresponding to higher energy (335-380 nm) is due to the π-π* transition. D149 layer was deposited on top of P3HT: PCBM to absorb photons which were not absorbed by the P3HT: PCBM active layer and therefore enhances the light-absorbing capacity especially in the range of 500-550 nm of the organic devices. This absorption increases both the number of collected photons and the number of created photo-electrons at photo-active/photo-cathode interface, which will increase the photocurrent of the all-small-molecule organic solar cells.

Fig. 2. Optical absorption of: P3HT:PCBM (solid line) and D149 (dashed line) thin film.

The I-V characteristics of the ITO/ PEDOT:PSS/ P3HT: PCBM or P3HT: PCBM / D149/ BCP /Al organic photovoltaic devices are plotted in the dark and under AM 1.5 (1000W/m²) irradiance in Figure 3. It can be observed that the structures exhibit diode behavior and a photovoltaic effect is clearly visible. We also have calculated the values of the shunt resistance and the series resistance (Table 1). For ITO/ PEDOT:PSS/ P3HT: PCBM / BCP /Al device, we have a VOC of 0.56 V, an ISC of 9.5 mA/cm² and a fill factor FF of 0.61, giving power conversion efficiency (PCE) of 3.24 %. In the case of ITO/ PEDOT:PSS/ P3HT: PCBM / D149/ BCP /Al, we have a VOC of 0.59 V, an ISC of 9.68 mA/cm² and a fill factor of 0.79, giving power conversion efficiency of 4.51 %. Under AM 1.5 (1000W/m²) irradiance, we can note that the D149 light absorbing layer improves the photovoltaic properties of the all-small-molecule organic solar cells. The insertion of this thin film smoothens the active layer surface and improves the photo-active/photo-cathode interface, which, on one hand, increases the shunt resistance R_sh from 769 to 1665 Ω.cm² and on the other hand, reduces the series resistance R_s from 13 to 5 Ω.cm².

Fig. 3. I/V characteristics of ITO/ PEDOT:PSS/ P3HT: PCBM/ BCP /Al (dashed line) and ITO/ PEDOT:PSS/ P3HT: PCBM /D149/ BCP /Al (solid line).

Figure 4 illustrates the structure and energy diagram of the All organic photovoltaic devices based on ITO/ PEDOT:PSS/ P3HT: PCBM /D149 /BCP / Al. First, we have absorption of
light and generation of excitons at the conjugated polymer P3HT. Then, the excitons separation at the bulkheterojunction interface, therefore, electrons are transferred from the LUMO of PCBM to the LUMO of D149 and holes are transferred from the HOMO of P3HT to the ITO/ PEDOT:PSS photoanode.

Using BCP improves the collection of electrons from the P3HT: PCBM/ D149 active layer to the cathode. Superior solar cell performance of the P3HT: PCBM/ D149/ BCP/ Al compared with that of P3HT: PCBM/ BCP/ Al structure is due to efficient light absorption and a better charge separation at the BCP/ Al cathode and active layer interface. By inserting the D149 light absorbing layer, photovoltaic characteristic values Voc, Isc and PCE are increased from 0.56 to 0.59 V, from 9.5 to 9.68 mA/cm² and 3.24 to 4.51 %, respectively.

### Tables

**Table I. All organic photovoltaic devices performance.**

<table>
<thead>
<tr>
<th>Active layer</th>
<th>Isc (mA/cm²)</th>
<th>Voc (V)</th>
<th>FF (%)</th>
<th>PCE (%)</th>
<th>Rs (Ωcm²)</th>
<th>Rsh (Ωcm²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>P3HT: PCBM</td>
<td>9.5</td>
<td>0.56</td>
<td>0.61</td>
<td>3.24</td>
<td>13</td>
<td>769</td>
</tr>
<tr>
<td>P3HT: PCBM/ D149</td>
<td>9.68</td>
<td>0.59</td>
<td>0.79</td>
<td>4.51</td>
<td>5</td>
<td>1665</td>
</tr>
</tbody>
</table>

### IV. CONCLUSIONS

We have prepared All organic photovoltaic devices based on P3HT: PCBM and D149 active layer and have evaluated their photovoltaic performance. Bathocuproine (BCP) was used as a buffer layer to block the diffusion of holes from the P3HT: PCBM/ D149 active layer to the cathode. Superior solar cell performance of the P3HT: PCBM/ D149/ BCP/ Al cathode and active layer interface. By inserting the D149 light absorbing layer, photovoltaic characteristic values Voc, Isc and PCE are increased from 0.56 to 0.59 V, from 9.5 to 9.68 mA/cm² and 3.24 to 4.51 %, respectively.

Figures and Tables

**REFERENCES**