



Molecular Crystals and Liquid Crystals

Publication details, including instructions for authors and subscription information:

<http://www.tandfonline.com/loi/gmcl20>

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Version of record first published: 22 Sep 2010

To cite this article: Seong-An Lee, Ki-young Ju, Je-jung Yun, Sung-Hoon Kim, Hee-Sung Ahn & Eun-Mi Han (2008): Bulk Heterojunction Photovoltaic Cells Based On Poly(3-hexylthiophene) and Pyran-4-ylidene-2-cyanoacetate Derivative, Molecular Crystals and Liquid Crystals, 491:1, 240-246

To link to this article: <http://dx.doi.org/10.1080/15421400802330671>

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Bulk Heterojunction Photovoltaic Cells Based On Poly(3-hexylthiophene) and Pyran-4-ylidene-2-cyanoacetate Derivative

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The effects of organic dye, pyran-4-ylidene-2-cyanoacetate derivative, and annealing on the dye-doped bulk heterojunction photovoltaics (PV) based with poly(3-hexylthiophene) (P3HT) and 1-(3-methoxycarbonyl)-propyl-1-(6,6)C61 (PCBM) have been investigated. The structures of the PV cells were ITO/PSS:PEDOT/P3HT:PCBM (1:1 wt. %)/Al and ITO/PSS:PEDOT/P3HT:PCBM:Pyran-4-ylidene-2-cyanoacetate derivative (1:1:0.5 wt. %)/Al electrode. Using the thermal treatment of the PV cell containing the organic dye at 140°C for 5 min, an increase in power conversion efficiency to 2.0% and external quantum efficiency (IPCE) to 36% are demonstrated.

Keywords: bulk heterojunction; cyanoacetate derivative; organic photovoltaic; PCBM; poly(3-hexylthiophene)

INTRODUCTION

Polymeric semiconductors have high potential for efficient production of low-cost flexible optoelectronics devices such as solar cells, photodiodes and light emitting diodes. Photovoltaics (PV) is one of

This work was supported by Korea Electrical Engineering & Science Research Institute.

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the most promising sustainable energy sources for the future, and organic solar cells have the potential to realize a significant cost reduction for PV energy conversion if improvements of the power efficiency and the lifetime can be achieved. The most common approaches to the highest efficiencies are organic bulk heterojunction (BHJ) formation within the photoactive layer using the conjugated polymers and fullerene derivatives, where efficient light-induced charge separation is enabled by large-area donor-acceptor interface [1–3]. Lately, several groups have published results demonstrating improved efficiencies to above 5% upon thermal annealing in P3HT:PCBM blends and these results show the importance of controlling the morphology in a BHJ device [4–6]. In this study, we have investigated the improvement of the PV characteristics through the incorporation of the P3HT:PCBM photoactive layer with the organic dye improving light harvesting and charge transport properties.

EXPERIMENTAL

The chemical structure of the materials and the configurations of PV cells used in this study are presented in Figure 1. The PV cells with

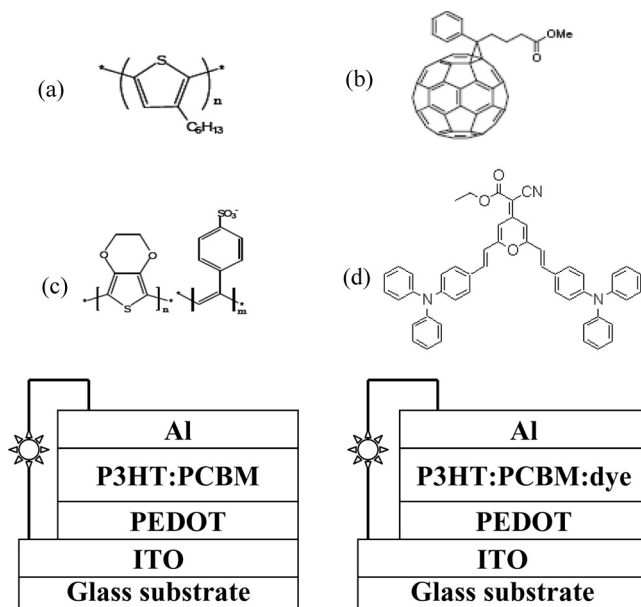


FIGURE 1 Chemical structure of materials and the configuration of PV cells used in this study.

a photoactive blend layer were fabricated based on conjugated polymer P3HT and fullerene derivative PCBM with or without pyran-4-ylidene-2-cyanoacetate derivative. The pyran-4-ylidene-2-cyanoacetate derivative dye has been synthesized and the P3HT and PCBM were purchased. The BHJ PV cells were prepared according to the following procedure. Solutions of the P3HT:PCBM and P3HT:PCBM:dye mixture were prepared with chlorobenzene in the optimized weight ratio of 1:1 and 1:1:0.5 wt.%, respectively. The thin film of poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) was formed on an indium-tin oxide (ITO) electrode by spin-casting at 3000 rpm and then dried at room temperature for an hour in a vacuum. Subsequently, the photoactive thin films were fabricated by spin coating technique at 3000 rpm from the chlorobenzene solution of the dye-doped and undoped P3HT:PCBM blend onto the PEDOT:PSS layer. Before the deposition of cathode, the prepared films were annealed at 80–155°C for 5–120 min. A high purity Al electrodes were deposited onto the photoactive film via thermal evaporation with the rate of deposition about 5 Å/sec and 100 nm thick. The active area of the PV cell is 0.25 cm².

The absorption spectra were measured with UV-visible spectrophotometer. The current density–voltage (J-V) characteristics of the PV cell were measured on a programmable electrometer with current and voltage sources (Keithley 2400) under an illumination of 92 mW/cm² (AM 1.5 solar simulator). The incident photon to current conversion efficiency (IPCE) was measured as a function of wavelength from 360 to 800 nm (PV measurement Inc.) equipped with a halogen lamp as a light source, and calibration was performed using a silicon reference photodiode.

All measurements and annealing of devices were performed under an air atmosphere.

RESULTS AND DISCUSSION

The absorption spectra of P3HT, PCBM and pyran-4-ylidene-2-cyanoacetate derivative, and their blend solutions are presented in Figure 2. The absorption maximum of P3HT and pyran-4-ylidene-2-cyanoacetate derivative can be observed at 451 nm and 477 nm, respectively. It is observed that there is a broad absorption peak at 478 nm in P3HT:PCBM (1:1 wt.%) blend, which shifts towards longer wavelength to 507 nm in the dye-doped blend.

Prior to the deposition of Al electrode, the photoactive P3HT:PCBM or P3HT:PCBM:dye blend films were annealed at 80, 100, 140 and 155°C for different times. Figure 3 shows the current density versus

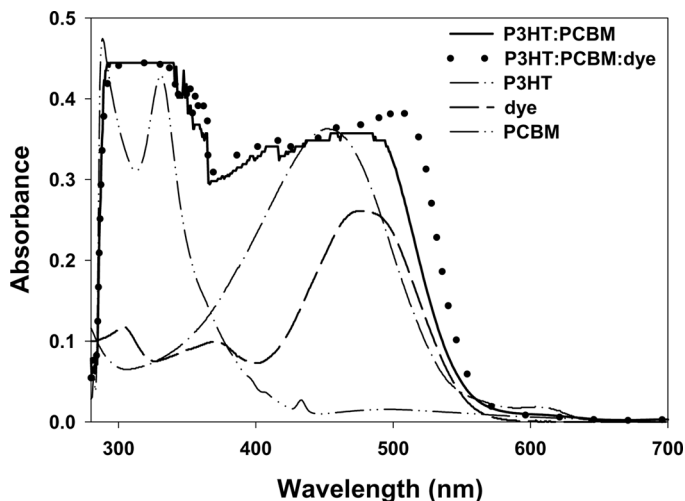


FIGURE 2 Absorption spectra of the pure and the P3HT:PCBM(1:1 wt.%) and P3HT:PCBM:dye (1:1:0.5 wt.%) blend solution

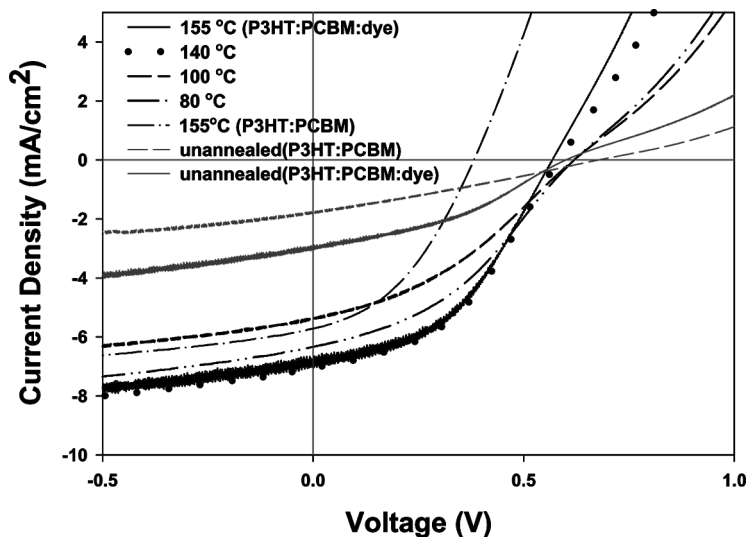


FIGURE 3 Current density versus voltage characteristic of the PV cells with the photoactive layer annealed at different temperature for the time showing maximum efficiency. The cell structures are ITO/PEDOT:PSS/P3HT:PCBM (1:1 wt.%) /Al and ITO/PEDOT:PSS/P3HT:PCBM:dye (1:1:0.5 wt.%) /Al.

TABLE 1 Photovoltaic Response of ITO/PEDOT:PSS/P3HT:PCBM (1:1 wt.%) Al and ITO/PEDOT:PSS/P3HT:PCBM:dye(1:1:0.5 wt.%) Al, Annealed at Different Temperature and for the Time Showing Maximum Efficiency Individually

Temp (°C)	Time (min)	J_{sc} (mA cm ⁻²)	V_{oc} (V)	FF	η (%)
ITO/PEDOT:PSS/P3HT:PCBM/Al					
No annealing	—	1.780	0.678	0.28	0.4
155	5	5.720	0.382	0.40	1.0
ITO/PEDOT:PSS/P3HT:PCBM:dye/Al					
No annealing	—	3.010	0.600	0.37	0.7
155	5	6.740	0.567	0.46	1.9
140	5	7.050	0.583	0.44	2.0
100	10	5.390	0.619	0.36	1.3
80	120	6.340	0.620	0.38	1.6

Active area 0.25 cm², AM 1.5 and 92 mW cm⁻², annealed in air.

voltage characteristics of the PV cells with the photoactive layer non-annealed or annealed at different temperature for the time showing maximum efficiency individually, which results are given in Table 1.

Without regardless to heat treatment of the photoactive films, the PV cell with the P3HT:PCBM:dye blend exhibits the better PV performance than the cell with the P3HT:PCBM layer. The higher annealing condition at 140°C and 155°C results in a higher J_{sc} and an overall higher efficiency. From Table 1, it can be seen that the overall power conversion efficiency increases from 0.4% to 0.7% by adding the pyran-4-ylidene-2-cyanoacetate derivative without annealing thermally, and from 0.7% to 2.0% when the P3HT:PCBM:dye blend film was annealed at 140°C for 5 min within this study condition.

Figure 4 shows the influence of the duration of the annealing on power conversion efficiency at different annealing temperatures. It has previously been shown by several groups in the literature that the efficiency of P3HT:PCBM blend PV cell is increased when the device is annealed thermally [4–8]. For the lower-temperature annealed devices at 80°C, the performance continues to rise with annealing time. However, the device with the dye shows the best power conversion efficiency within 5 min when annealed at 140 and 155°C, which shows 5-fold enhanced efficiency in comparison with the P3HT:PCBM blend cell even though annealed under an air atmosphere.

In Figure 5 the results of the IPCE measurements for all three kinds of devices are shown. The external quantum efficiency for the as-produced device with the dye (triangles) shows a maximum of

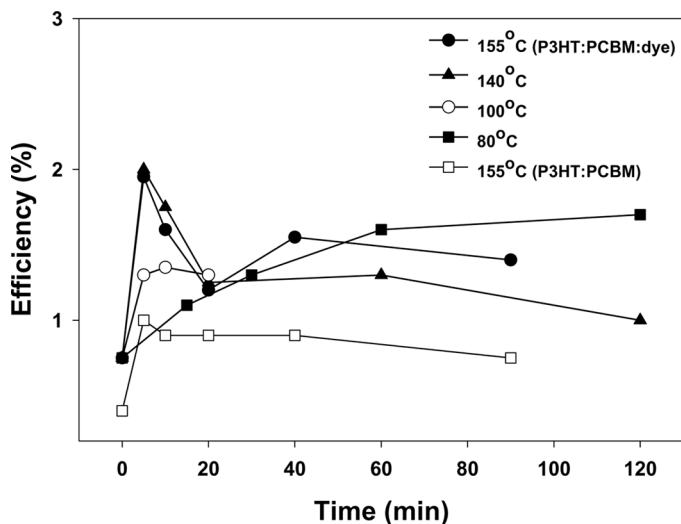


FIGURE 4 Influence of the duration of the annealing on power conversion efficiency at different annealing temperature.

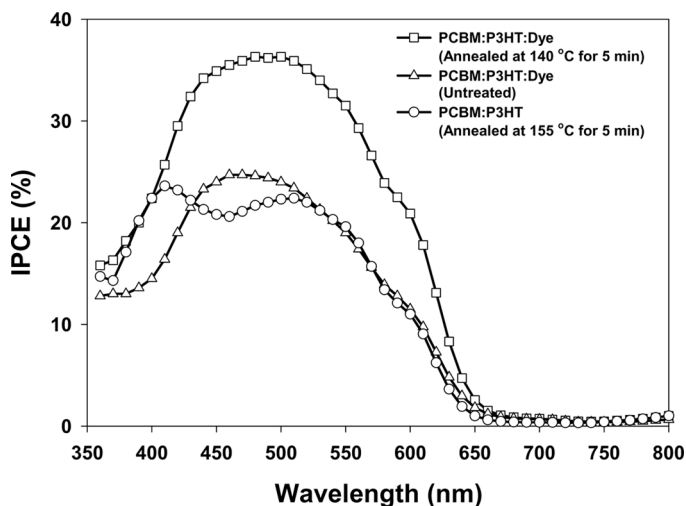


FIGURE 5 The comparison of incident photon to current conversion efficiency (IPCE) spectra of P3HT:PCBM and P3HT:PCBM:dye-based devices.: P3HT:PCBM annealed at 155°C for 5 min (circles), as-produced P3HT:PCBM:dye (triangles), and P3HT:PCBM:dye annealed at 140°C for 5 min (squares).

~25% at a wavelength of 465 nm, which shows the similar maximum of the IPCE in comparison with the P3HT:PCBM blend cell treated at 155°C for 5 min (circles). Using a thermal treatment of the PV cell with the dye at 140°C for 5 min, the IPCE is increased to ~36% (squares), while the maximum is shifted to a wavelength of 490 nm. Therefore, we presume this enhancement of the IPCE is originated from an enhancement of the charge carrier mobility of the bulk.

CONCLUSIONS

We have presented the effects of the incorporation of the pyran-4-ylidene-2-cyanoacetate derivative in a P3HT:PCBM PV device and the annealing of the photoactive films. Using a thermal treatment at 140°C for 5 min of the PV cell with the organic dye, PV cells with an IPCE above 36% and a power conversion efficiency of around 2.0% under irradiation intensity of 92 mWcm⁻² were produced, which is presumed to result from an increase of the charge carrier mobility.

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