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Solvent Effects on Performance of P3HT: PCBM Organic Solar Cell

Mohammed T. Obeed

Department of Material Science, Polymer Research Centre, University of Basrah

***E-mail: mhamdto@yahoo.com**

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Abstract

Regioregularpoly(3-hexylthiophene)(P3HT):[6,6]-phenylC61-butyricacidmethylester (PCBM) active layer were found to significantly increase organic solar cell performance. photovoltaic devices with three solvents, Toluene (T), Xylene (X), and co-solvent Toluene:Xylene (T:X) were fabricated. The physical properties of these devices with different solvents are investigated. In this paper, we find that, absorption spectrum of the blend becomes more broad with different solvents, which is highly desirable for photovoltaic devices. Films morphology is evaluated by Atomic Force Microscopy (AFM). X-Ray diffraction (XRD) samples and External Quantum Efficiency (EQE) measurements are also performed for the active layers. The Power Conversion Efficiency (PCE) enhancement for the device with (T:X) is more significant than for other solvents. With different solvents, the solar cells upon (T:X) give (PCE) of 0.176%, in contrast to 0.144% for (T), and 0.079% for (X), devices.

Keywords: P3HT:PCBM, Organic, Solar Cell, toluene, Xylene.

1. Introduction

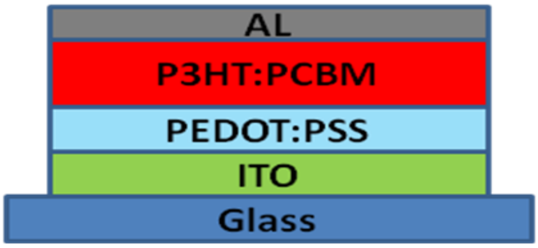
Converting solar energy into electrical energy is becoming significant due to the crisis in conventional energy sources nowadays. There are different natural resources available to generate energy. Converting solar energy into electrical energy is one of such exploitation of the natural sources. Inorganic solar cells are the best utilized for the last few decades in this direction[1, 2]. But, the drawbacks such as manufacturing high costs and difficult fabrication process made researchers to look into easily processable nature and low cost polymer materials. Many work have been done for almost last one decade on polymer solar cells, but the lower power conversion efficiency (PCE) limits their commercial usage [1–10]. After introduction of bulk-heterojunction concept, the PCE of polymer solar cells is nearing to 5% [7–10]. But, these values are not sufficient to meet realistic specifications for commercialization.

The formation of bulk-heterojunction phase allows for bulk separation of photoinduced excitons and high-mobility removal of electron through the nano-phase. Poly(3-hexylthiophene) (P3HT) has been the mostly used p-type material [7–10] in polymer solar cells along with a fullerene derivative, [6,6]-phenyl C61-butyric acid methyl ester (PCBM) as an electron acceptor. Since hole is typically the high-mobility carrier in regioregular P3HT [11], the enhanced electron mobility was achieved by addition of electron acceptor. However, the difficulty in these systems arises when we account for the effects of morphological modifications in P3HT phase due to the introduction of nano-phase [1, 12]. There are significant number of studies that investigate the effects of processing parameters on blended photoactive nano-phase [12–16]. Even, the regioregularity and molecular weight [17, 18] of P3HT also affect the performance of P3HT:PCBM devices. The electric power extracted from a photovoltaic device depends on both the photocurrent and photovoltage of the diode under illumination of a given intensity. In order to increase the PCE of a photovoltaic device, the practicable approach is to increase the photocurrent as much as possible, since the solar cell is limited by the built-in potential and it is the difference between the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) of the electron donor and acceptor materials [19]. Different device geometries and interface morphologies are evaluated for the purposes of trapping more light, dissociating excitons more efficiently, transporting charges with fewer impediments in order to extract more photocurrent [20]. Indeed, the solvents used for the preparation of active layer have shown a strong impact on its morphology, which influences the generation of photocurrent in the devices [15, 16]. Unfortunately, till to date no conclusive result was made for optimal processing of the nanophase.

2. Experimental Work

2.1. Photovoltaic device fabrication

Pre-patterned indium tin oxide (ITO)-coated glass slides (120 nm thick and, 10Ω/sq sheet resistance as received). The ITO substrates were first cleaned with isopropyl alcohol for 20 min, the heat dried in an oven at 125^0C. A film of PEDOT: PSS: was spin cast on top of the ITO substrates with a speed of 3000 r/min for 30 s to form the hole-transport layer, and was dried for 20 min at 120 ^{0}C. Afterwards, the mixed solutions consisting of P3HT: PCBM (10 mg mL^{-1}: 10 $mgmL^{-1}$ Sigma-Aldrich) in different solvents (T), (X), and (T:X) in 1:1 weight ratio, then spin coated at 1000 r/min for 30 s on the buffer layer film to form the active layer. The thickness of the active layer is ~140 nm and thickness of the buffer layer (40 nm) . Finally, after 24h, a bilayer cathode consisting of 80 nm (Al ~ 99% pure) was thermal evaporated under high vacuum of ~ 2×10^{-6} torr with a rate of 0.2 nm/s onto the polymer layer as a cathode to create a device with an active area of 9 mm^2 defined by a shadow mask on the active layer to form cells with an active area of 1 cm^2 .



Organic Solar Cell Devise.

2.2 Device characterization

The current density–voltage (J–V) characteristics of devices were measured with a computer-programmed Keithley 2400 Digital Source Meter and the photocurrent was generated under AM 1.5 G irradiation of 100 mWcm^{-2}. P3HT:PCBM films were prepared by spin coating P3HT:PCBM solution on glass substrates for UV–vis absorption spectroscopy and atomic force microscopy (AFM).The UV–vis absorption spectra of the polymer films were taken with a Varian Cary 5000UV– VIS–NIR spectrometer and Raman spectroscopy using a Horiba Jobin Yvon HR800 micro-Raman spectrometer. The light intensity for the solar simulator was calibrated with a standard photovoltaic (PV) reference cell. The AFM images of the polymer films were acquired using a BRUKER NanoScope IV Multi-Mode Adapter AFM with the tapping mode. The film thickness was determined with aTencorP-10 Alpha-Stepprofiler. The PCE is described by $\eta = FF \times (V_{oc} \times J_{sc})/P_{light}$, where the FF (fill factor) is defined as $FF = (I_{max} \times V_{max})/(I_{sc} \times V_{oc})$ and the P_{light} is the power of incident light.

3. Results and Discussion

Figure (1) shows the UV–vis absorption spectra of P3HT:PCBM film prepared from different solvents. An interesting effect was observed, the P3HT:PCBM prepared from the (T:X) co-solvent showed the maximum absorption intensity and shifting in the wavelength in the visible wavelength in ranging around (400- 650 nm) compared to the other samples. It is observed that, the absorption intensity of the P3HT:PCBM films are affected by the solvent species, indicating that a large number of photons are absorbed in the bulk heterojunction dissolved by the (T:X) co-solvent. It is expected that the high value of the light absorption intensity could lead to an improvement and increase in the generation rate of (e-h) excitons. This result can also be explained by a change in the stacking conformation of the polymer structure from high crystallinity to lower crystallinity, and a reduction of intraplane and interplane stacking, which causes a poor π–π* transitions and lower absorbance [21,22]. The portion of the spectra in the wavelength range lower than 400 nm for all solvents corresponds to the absorption of PCBM [23].

Figure (2) shows the XRD results from bulk heterojunction of P3HT:PCBM prepared by spin coating from various solvents of (T), (X), and (T:X), respectively. The XRD intensity values were obtained peaks at $2\theta \approx 5.4$ for all solvents, where the reflection of (d_{100} -spacing) plane correspond to as describe by the (JCPDS 44-0558) [21]. These values are corresponding to the inter-chain spacing in P3HT associated with the interdigitated alkyl chains and indicating the degree of crystallinity of P3HT [24, 25]. In the case of mixed solvents, P3HT undergoes competitive film growth rate during spin-casting from solvents with two different vapor pressure and solubility. The P3HT in the bulk heterojunction prepared from a mixed solvent (T:X) is obtained more improved crystallinity than mono solvent such as T and X. However, crystallinity of P3HT was not improved when the bulk heterojunction prepared from a mixed solvent (T:X) because T and X have too different vapor pressure to occur competitive growth rate [25-27].

The microstructure of the P3HT:PCBM blends by using (T), (X), (CF), and (T:X) as solvents were studied using the atomic force microscopy (AFM) technique. Figure (4) shows the surface morphologies measured using AFM for the P3HT:PCBM Bulk heterojunctions prepared from the various solvents. The root-mean- square (R.M.S) for the Bulk heterojunctions dissolved with the various solvents such as the T, X, and T:X co-solvents, were found to be 3.64, 3.81,and 4.22 nm, respectively. These results indicate that the P3HT:PCBM bulk heterojunction prepared from the T:X co-solvent has a coarser film surface morphology compared to the samples since it shows a higher R_{max} value of 4.22 nm. This rough film surface results in a large surface area and so leads to an improved efficiency in the charge generation through the effective incidence of the photons. The rough film surface is probably the signature of a polymer self-organization, which in turn enhances the ordered structure formation found in the thin film [28]. This ordered structure reduces the internal series resistance of the device, thus increasing the photocurrent [28]. It may be noted that the evaporation rates and the solubility of the solvents can affect the surface morphologies of the polymer bulk heterojunctions. By mixing both solvents together, the evaporation rate of the co-solvent is modified, resulting in different surface morphologies. In addition, the solvating activation energy also significantly influences the morphology of the films, because a good solvent may produce a better extension of the polymer chain in a solid state thin film. Considering the results of the surface morphologies as they are affected by the various solvents, a high vapor density, a low solubility, and the evaporation rate in the T solvent, as shown in Table (1), lead to a rough film surface when they are spin coated on the P3HT:PCBM film and post-annealed at 125 ^{o}C.

Figure (4) shows the EQE values of P3HT:PCBM films prepared from different solvents, such as the (T), (X), and (T:X) co-solvents. It was observed that the P3HT:PCBM films prepared from the T:X co-solvent showed the highest peak external quantum efficiency value in the wavelength range from ~ 400 to 600 nm. From this result, we conjecture that the external quantum efficiency values may be related to the absorption results show that the T:X blend layer absorb significantly stronger than that of all solvents [29]. The highest peak of external quantum efficiency value can be attributed to the crystalline property as well as the surface morphology of P3HT:PCBM films.

Figure (5) shows the current density versus voltage (J-V) characteristic curves and device parameters of the parameters short-circuit current density (J_{sc}), open-circuit voltage (V_{oc}), fill factor (*FF*) and power conversion efficiency (*PCE*) values of the organic solar cells with P3HT:PCBM prepared from the various solvents. The parameter values for the PEDOT:PSS/P3HT:PCBM film dissolved with the various solvents such as the T, X, and T:X, co-solvents. The maximum parameters (J_{sc}), (V_{oc}), and (*FF*) values were found to be 0.72 mA/cm^2, 0.5 mV and 0.45, respectively for the PEDOT:PSS/P3HT:PCBM film using the T:X co-solvent, indicating that the *PCE* calculated to 0.176. From our experiments, it may be concluded that the observed improvement in the electrical properties of the organic solar cells with the PEDOT:PSS/P3HT:PCBM film dissolved with the T:X co-solvent is caused by a favorable change in the enhanced crystallinity, the absorption light intensity, and the rough surface morphology of the bulk heterojunction due to the high vapor density and low solubility of the mixing solvents [30, 31]. The (J_{sc}), (V_{oc}), and (FF) values of the organic solar cells with P3HT:PCBM bulk heterojunctions prepared from the various solvents such as pure and co-solvents are summarized in Table 2.

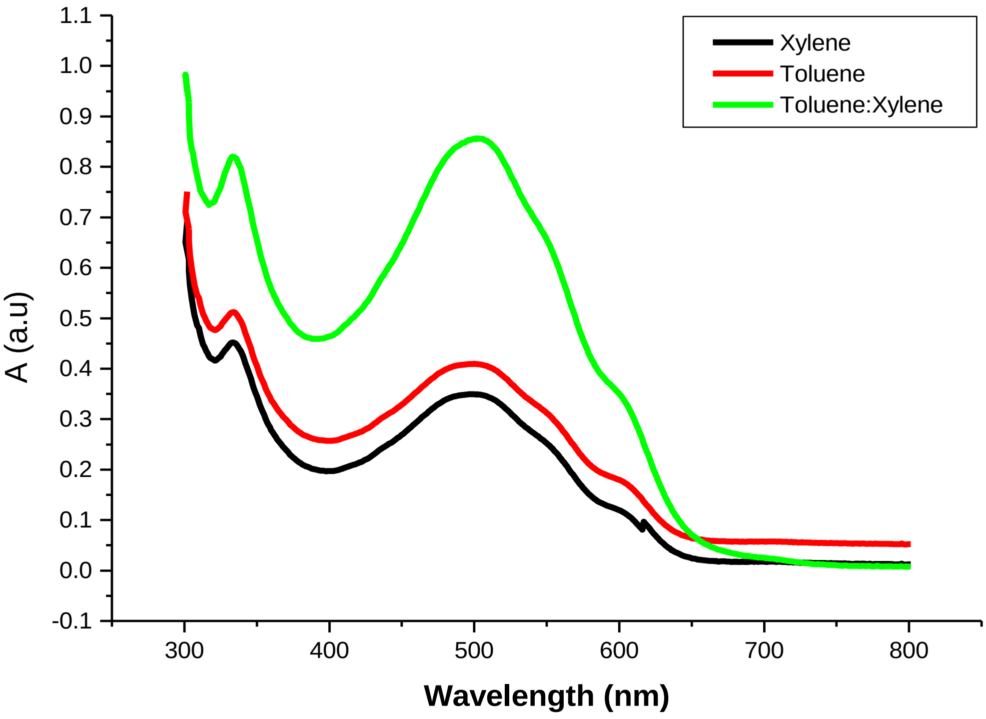


Figure 1: UV–vis absorption spectra for P3HT:PCBM films with different solvents (T), (X), and (T:X).

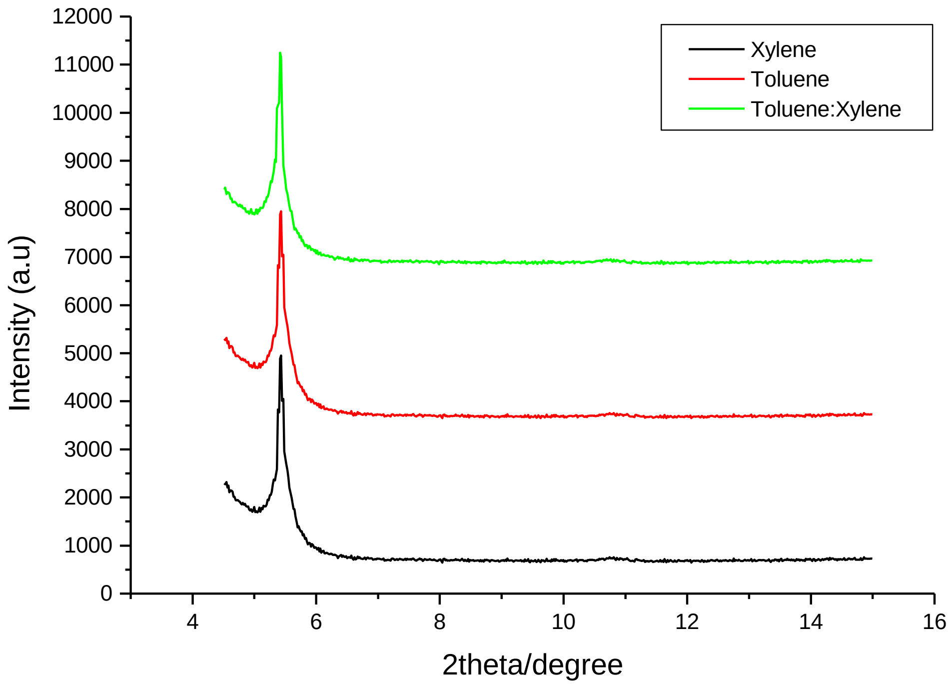


Figure 2: XRD curves for for P3HT:PCBM films with different solvents (T), (X), and (T:X).

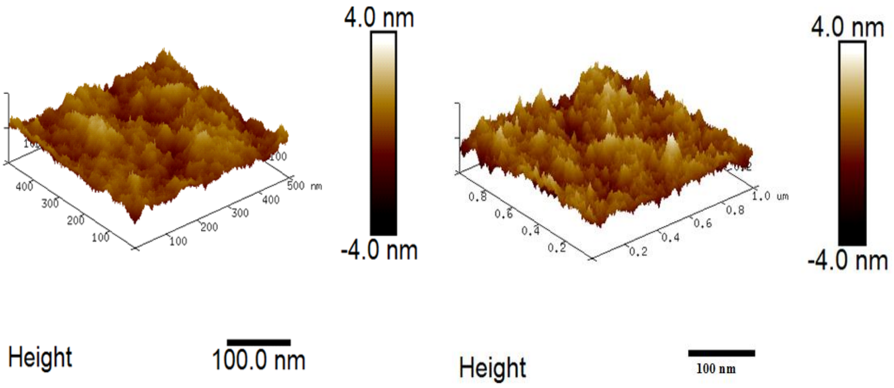


Figure 3: AFM images of for P3HT:PCBM films with different solvents (T), (X), and (T:X).

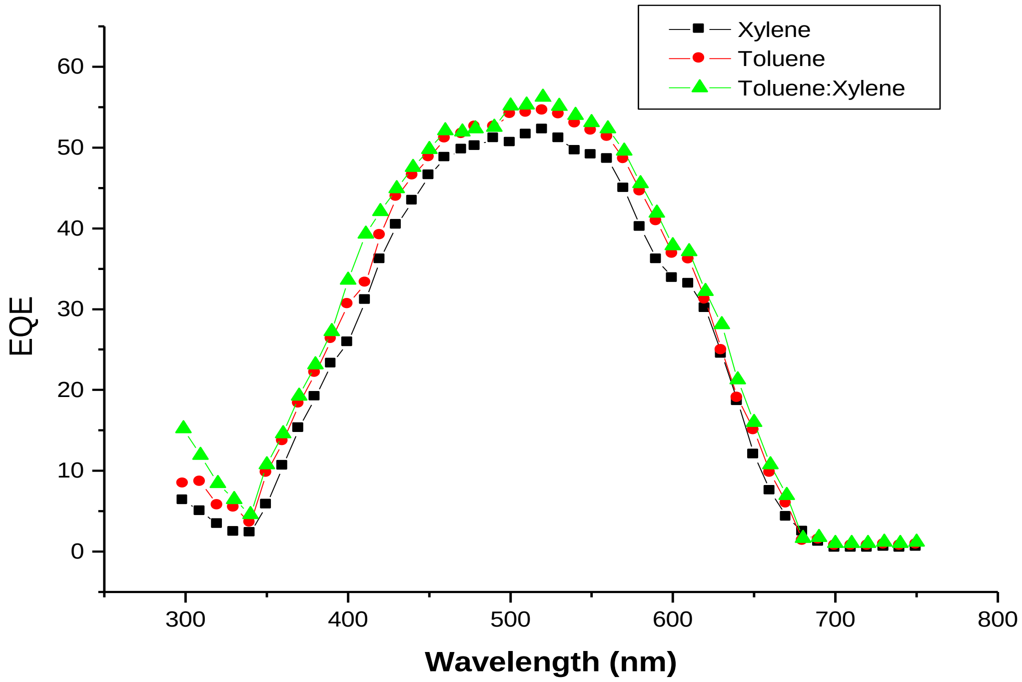


Figure 4: EQE spectra of for P3HT:PCBM films with different solvents (T), (X), and (T:X).

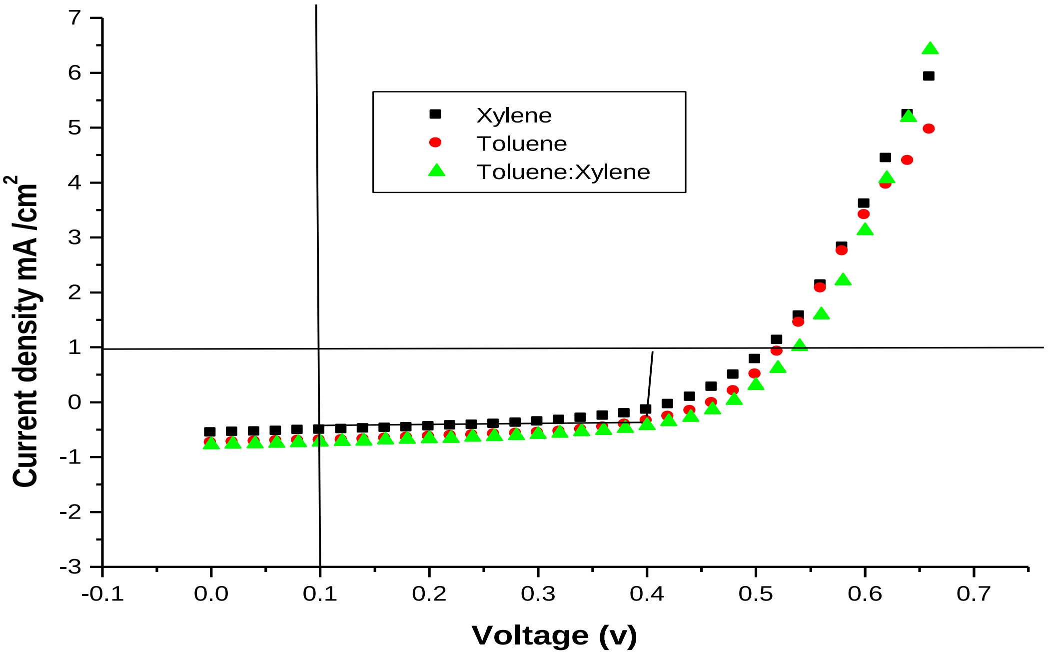


Table 1. AFM value of P3HT:PCBM film with different solvents (T), (X), and (T:X).

solvent	R.M.S (nm)	R_a(nm)	R_{max}(nm)
Toluene	3.64	3.04	19.3
Xylene	3.81	3.32	27.4
Toluene:Xylene	4.22	4.11	34.2

Table 2. Photovoltaic parameters for PEDOT:PSS/P3HT:PCBM films with different solvents (T), (X), and (T:X).

Devices	V_{oc} (v)	J_{sc} (mA/ cm^2)	FF	PCE (%)	R_s (Ω cm^{-2})	R_{sh} (Ω cm^{-2})
Toluene	0.51	0.48	0.38	0.079	9. 3	826
Xylene	0.52	0.63	0.45	0.144	12. 7	883
Toluene:Xylene	0.53	0.72	0.49	0.176	12.6	721

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تاثير المذيبات على كفاءة الخلية الشمسية العضوية

محمد توفيق عبيد
جامعة البصرة ، مركز ابحاث البوليمر، قسم علوم المواد

الخلاصة:

صنعت في هذا البحث خلايا شمسية عضوية من(البولي هكساثايوين : فوليرين 61) باستخدام ثلاث مذيبات هي التلوين والاكزايلين ومذيب مشترك من(التلوين:الاكزايلين). درست الخواص الفيزيائية للخلايا المحضرة ، وبينت ان هنالك تحسن ملحوظ في كفاءة الخلية المصنعة باستخدام المذيب المشترك (التلوين:الاكزايلين)، كذلك درست خواص سطوح الاغشية المحضرة باستخدام تقنيتي مطياف القوة الذرية وتشتت الاشعة السينية. كما درست كفاءة الكم الخارجية ووجد ان الخلية المحضرة باستخدام المذيب المشترك (التلوين:الاكزايلين) افضل من الخليتين المحضرتين باستخدام التلوين والاكزايلين. وجد كذلك ان كفاءة الخلية المحضرة باستخدام المذيب (التلوين:الاكزايلين) هي 0.176% مقارنة بخلية مذيب التلوين 0.144% وخلية مذيب الاكزايلين 0.079%