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Influences of CdSe NCs on the photovoltaic parameters of BHJ organic solar cells



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ABSTRACT

In this study, the high quality CdSe nanocrystals (NCs) capped with stearic acid were synthesized in a solvent and then purified four times by using the precipitation and redissolution process. The average size of the synthesized CdSe NCs was determined ~3.0 nm via transmission electron microscopy (TEM) measurement and their corresponding optical band edge energy was also calculated as ~2.1 eV using ultraviolet-visible (UV-Vis) absorption spectroscopy. The bulk heterojunction (BHJ) hybrid solar cells based on a ternary system including P3HT, PCBM and CdSe NCs at different weight concentrations (0 wt%, 0.1 wt%, 0.5 wt%, 1 wt% and 2 wt%) were fabricated by spin-casting process. The effect of the concentration of CdSe NCs on the photovoltaic parameters of these BHJ organic solar cells was investigated. The surface morphology of the photoactive layer modified by the incorporation of CdSe NCs into P3HT:PCBM matrix was observed with scanning electron microscopy (SEM). It was shown that when the concentration of CdSe NCs increases above 0.1 wt% in this ternary system, the photovoltaic performance of the devices significantly decreases. The power conversion efficiency of the organic photovoltaic (OPV) device was enhanced ~20% by incorporating CdSe NCs with 0.1 wt% with respect to those without CdSe NCs.

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1. Introduction

Excessive consumption of fossil fuels (a non-renewable energy resource) such as coal, crude oil and natural gas causes to harmful impacts on the environment. Some of these harmful effects are climate change as a result of global warming, air pollution and toxic wastes. Organic photovoltaic (OPV) solar cells have attracted enormous attention because of growing demand for renewable energy sources. OPV solar cells offer a variety of advantages like low manufacturing cost and easy handling and processing [1–4]. On the other hand, there are some disadvantages like lower efficiency and shorter lifetime as compared to inorganic ones. Therefore, new electron acceptor and donor materials are especially needed to enhance the efficiency of OPV solar cells. The concept of the bulk heterojunction (BHJ), based on a nanoscale blend of a conjugated polymer as an electron donor and a fullerene derivative as an electron acceptor material, comes into prominence to increase the efficiency of organic solar cells by way of providing a charge-separating network throughout the absorption layer, because the exciton diffusion lengths are generally very short in organic semiconductors [5–8]. The Poly(3-hexylthiophene) (P3HT) which is widely used in many organic electronic applications because of its unique properties

have been mostly investigated. The power conversion efficiency of the BHJ with the blends of poly(3-hexylthiophene-2, 5-diyl) (P3HT) and [6,6]-phenyl C61 butyric acid methyl ester (PCBM) has approached to 4% [9–11].

Hybrid solar cells comprising of conjugated polymers and inorganic semiconductor nanocrystals are of great interest in the literature of third generation solar cells due to the high electric permittivity and low binding energy within the inorganic component to reduce the energetic driving force for charge separation. However, the poor, hopping type electron transport in the inorganic component of binary hybrid solar cells employing inorganic nanocrystals and conjugated polymers and also the requirement for high nanocrystals loading of the polymer to reach the percolation threshold are the main drawbacks towards higher efficiencies [12]. On the other hand, the surfactant, which prevents the further growth of nanocrystals, is an insulating layer, which blocks the electrical transport between the nanocrystals. Therefore, tailoring of such surfactants is an important issue [13]. For their efficient use in hybrid solar cells organic ligand shell surrounding the nanocrystals needs to be removed. Ligand exchange route is followed in the literature [14]. However, it has some disadvantages such that it can cause a tendency of the nanocrystals to form large aggregates, which may affect the charge transfer and morphology in hybrid solar cells. In hybrid polymer/CdSe solar cells chlorobenzene/pyridine or chloroform/pyridine binary solvents are used, if the ligand shell of

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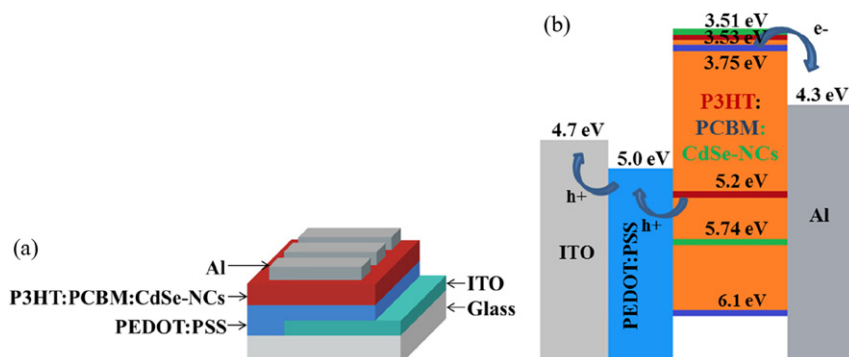


Fig. 1. Schematic description of the device structure with Glass/ITO/PEDOT:PSS/P3HT:PCBM:CdSe-NCs/Al (a) and its energy level diagram (b).

nanocrystals is replaced by pyridine, as a result the film morphology becomes dependent on binary solvent ratio.

Inorganic semiconductors such as CdSe, CdS and CdTe have a high dielectric constant, high charge mobility and high light absorption. So, hybrid solar cells comprising of these inorganic semiconductors or their nanocrystals and organic materials are of great interest thanks to providing advantages of both materials [15–16]. CdSe nanocrystals (NCs) having different shapes like rods, tetrapods have used as electron acceptors with electron donor polymers in hybrid solar cells [17–19]. Long chain fatty acids such as oleic acid (OA) and stearic acid (SA) are used often to passivate surfaces of the nanocrystals successfully. However, they must be removed from the surfaces of the nanocrystals as much as possible or replaced with short chain ligands using ligand exchange reactions to improve their charge transport [20–21]. The most commonly used method for purification of nanocrystals is precipitation and redissolution process. The purification process of long chain fatty acid stabilized CdSe NCs also helps to improve the efficiency of BHJ solar cells [22–23].

In previous studies, the hybrid solar cells involving CdSe NCs which act an electron acceptor and P3HT which acts an electron donor have been mostly investigated for binary systems but not that much for ternary systems including PCBM [24–29]. In this research, CdSe NCs capped with stearic acid were synthesized by using hot injection method [30]. Then, CdSe NCs were purified via successive precipitation from methanol and finally stored in chlorobenzene (CB). We fabricated BHJ organic photovoltaic based on a ternary system consists of a blending of P3HT, PCBM and CdSe NCs. The structure of photovoltaic device consisting of ITO/PEDOT:PSS/P3HT:PCBM:CdSe-NCs/Al was created and its photovoltaic parameters were measured depending on the various concentrations of CdSe NCs. The energy levels of CdSe NCs having LUMO ~ 3.5 eV and HOMO ~ 5.7 eV are suitable for LUMO energy level of PCBM ~ 3.8 eV and HOMO energy level of P3HT ~ 5.2 eV. The values

of the energy levels of materials used in this structure were taken from references [31–32]. Schematic description of the device structure and its energy level diagram are shown in Fig. 1.

Here, we used a simple centrifuging method to prepare dry CdSe nanocrystals and the novelty of this work lies in the fact that we were able to dissolve them in chlorobenzene without needing any binary solvent mixtures and we mixed these CdSe NCs in P3HT:PCBM blend to fabricate ternary hybrid solar cells. Our aim was to study the effect of CdSe NCs on optical, morphological and electrical properties of the active layer and also the power conversion efficiency of the devices.

2. Experimental

Indium Tin Oxide (ITO) coated substrates bought from Kintec Company which have a thickness of around 120 nm, a sheet resistance of 12 Ω /sq. and a size of 1.5×1.5 cm² were used as anode electrode. The one-third of ITOs was patterned by etching with an acid mixture (HCl:HNO₃:H₂O) and then each substrate was cleaned with Hellmanex™, distilled water, acetone and isopropanol in an ultrasonic bath for 20 min, respectively. The aqueous solution of poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS, Clevious PH1000) filtered with 0.45 μ m Whatman filter was deposited on top of the ITO substrates by spin coating at 1500 rpm for 60 s. The PEDOT:PSS coated samples were annealed in an oven at 150 °C for 4 min under atmospheric condition in order to remove residual moisture. The solutions used in purification process of CdSe NCs had been completely removed by centrifugation and drying and then pure CdSe NCs free of solvents was extracted. The purified CdSe NCs were dried under vacuum for evaporating their solvents and then obtained solid precipitate was weighed as 3.7 mg. This solid precipitate was dissolved in 4 ml CB to prepare a stock solution with a concentration of 0.925 mg/ml. The homogeneous stock solution

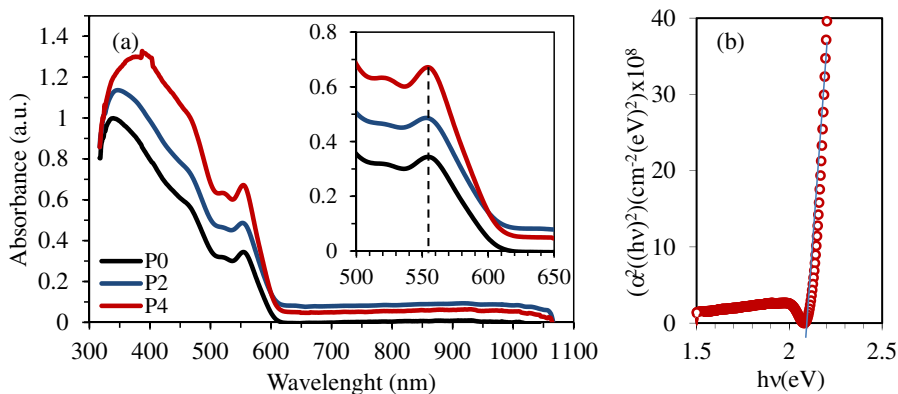


Fig. 2. (a) The absorption spectra of the synthesized CdSe NCs. The black curve labelled as P0 is the absorption spectrum of the unpurified CdSe NCs. The blue (P2) and red (P4) curves are the absorption spectra of the CdSe NCs purified for 2 times and 4 times, respectively. (b) Tauc plot of the purified CdSe NCs. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

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