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A Simple Method for Incorporating Lead Sulfide Nanoparticles Directly in Poly (3-hexyl thiophene) (P3HT) Matrix

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Abstract

In the present study, nanoparticles (NPs) of lead sulfide (PbS) have been directly incorporated in poly (3-hexylthiophene) (P3HT) matrix without any surfactant. The X-Ray diffraction and absorption spectrum confirm the incorporation of PbS NPs in P3HT matrix. The strong and sharp diffraction peaks indicate that the as-prepared PbS NPs are crystalline. The absorption spectrum of P3HT in solution shows a characteristic wide peak at 451 nm. The extension of the blend absorption beyond the main polymer exciton peak at ca. 451 nm is due to the presence of PbS nanoparticles. The broad photoluminescence in the visible spectral region from the P3HT-PbS blend is observed, which is very much dependent on the PbS concentration.

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Keywords: PbS NPs; P3HT; blend solution; organic photovoltaic devices

1. Introduction

Photovoltaic devices with an active layer composed of a conjugated polymer and semiconducting nanoparticles (NPs) are very attractive, as they take advantage of the tunability of the photophysical properties of the NPs, while retaining the solution processability offered by the polymer [1-5]. In these cells, the charge transfer takes place between polymer and nanoparticles because of built in potential due to different electron affinities of NPs and polymer. Until now researchers have synthesised the NPs

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capped with organic aliphatic ligands, such as trioctylphosphine oxide (TOPO) or oleic acid. These capping agents hinder the efficient electron transfer from the photoexcited polymer to the nanoparticles [6]. To remove the capping agents, polymer- NPs were treated with pyridine. However, pyridine is an immiscible solvent for semiconducting polymers and flocculation of the poly (3-hexylthiophene) (P3HT) chains in an excess of pyridine may lead to large-scale phase separation resulting in poor photovoltaic device performance [7].

To overcome the effects of organic ligands on charge transport we have directly grown PbS NPs in a conducting polymer solution without any surfactants or ligands [8]. Direct synthesis of nanoarticles in polymer matrix controls the dispersion of nanoparticle in organic phase. In addition, nanoparticles are uniformly distributed to the entire active area of the device and thus contains a built in percolation pathway for transport of charge carriers to the respective electrodes. It is normally understood that the in situ synthesis of the nanostructures (nanorods), in the polymer matrix is favourable for photovoltaic application because nanorods exhibit much better connectivity than spherical nanoparticles and act as large surface area electron acceptors in a bulk heterojunction [6]. In addition, because of two dimensions confinement, nanorods modifies the band structure resulting in the tunable optical absorption edge [6], while allowing exciton diffusion and separation along the unconfined dimension [9]. In surfactant-assisted synthesis, nanoparticles growth is controlled by electrostatic interactions of the surfactant functional group and steric hindrance of surfactant alkyl side chains. P3HT provides a combination of both effects as it contains an electron donating sulfur functionality, a potential anchorage for the nucleation, and growth of nanoparticles along with steric hindrance due to long hexyl side chains [10]. Direct synthesis of CdS nanorods and CdSe nanoparticles [10] in P3HT matrix have been reported previously. Because PbS have tunable bandgap for solar cells and also absorb infrared part of solar spectrum compared to the CdSe and CdS nanocrystals, hence replacement of theses nanocrystals with PbS would enable these hybrid devices to further enhance the power conversion efficiency.

Here we report the synthesis of PbS nanoparticles in P3HT matrix. The blend of P3HT and PbS, where lead acetate:sulfur is 1:1, is designated as P3HT11 and the polymer can be easily dissolved in same solvents for casting thin films. Optical measurements show that the photoinduced charge separation occurs at interface between the nanocrystals and polymer, this indicates a promising approach for the fabrication of efficient organic-inorganic hybrid photovoltaic devices.

2. Experimental Procedure

Lead acetate dihydrate and sulphur powder were employed as the precursors for PbS formation. Tri-chlorobenzene (TCB) and dimethyl sulfoxide (DMSO) were used as the solvents for PbS formation. P3HT11 is a blend of P3HT and PbS, where lead acetate:sulfur is 1:1.

In a three-neck round-bottom flask equipped with a magnetic stirring bar and condenser, 22 ml of TCB, 11 ml of DMSO, 300 mg of lead acetate dihydrate, and 30 mg of P3HT were heated to 180ºC and degassed with nitrogen for 30 min. In a second vial, 300 mg of sulphur was dissolved in 15 ml of anhydrous TCB at 180ºC and degassed with nitrogen for 60 min. Then, 15 ml of the sulphur solution was injected swiftly into the lead precursor solution. The solution was allowed to react for 30 min. The blend of PbS and conducting polymer was purified by removing any lead, sulphur ions, and DMSO via adding anhydrous methanol to form the precipitate. After centrifugation, the supernatant was removed and the composite dried in vacuum at 70ºC.

X-ray diffraction studies were done using Phillips X'PERT PRO having CuKα incident beam (λ= 1.54056). Absorption spectra were measured with a UV-Vis-NIR spectrophotometer (Perkin Elmer