

The influence of ionic radius of interfacial molecule on device performances of polymer solar cells



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ABSTRACT

Ionic radius of interfacial molecular can affect the interface property and key electron transfer processes occurring at interface in polymer solar cells. To study the effects of different ionic radius of electron transfer layer on device performances, we introduce various stearate salts (Na^+ , K^+ and Cs^+) as electron transfer layer to fabricate polymer solar cells. Interestingly, it is found that the key device parameters such as V_{oc} , J_{sc} , fill factor and PCE of polymer solar cells present regular change with the ionic radius increasing. We systematically study the effects of different ionic radius of electron transfer layer on the various parameters of polymer solar cells and believe this regularity paves a way for further understanding and improving the performances of polymer solar cells.

1. Introduction

Conventional polymer solar cells (PSCs) with an active layer sandwiched between transparent conducting electrodes have attracted great attention due to their advantages such as ease of fabrication, solution-based processing, low cost and the capability for large-area manufacturing technology at low temperatures (He et al., 2011; Lee et al., 2014; Wang et al., 2014a,b; Sun et al., 2014; Li et al., 2018a). In this device configuration, electron transfer layer (ETL) located between active layer and top electrode layer plays a crucial role in determining the performance of PSCs (Wang et al., 2016; Fan et al., 2017; Yu et al., 2017). Inserting an organic ionic salt as ETL between active layer and electrode layer was proved as a simple and effective method to fabricate high performance PSCs devices. Most of reports focus on the effect of backbone and morphology of organic ionic salts on the performance of PSCs, such as the nature of conjugated or non-conjugated of the backbone of organic ionic salts (Wang et al., 2017; Ouyang et al., 2015; Li et al., 2013; He et al., 2012; Zhang et al., 2015). Aside from these, it should be noted that the nature of the ion of organic ionic salts (such as the change of the ionic radius of organic ionic salts) can influence the carrier transport and collection occurring at interface as well and consequently affect the device performance (Li et al., 2016). However, the above investigations are still lacking, which has limited further development and application of polymer solar cells. Therefore a deep investigation and specification of the effect is vital for further

mechanism understanding and performance improvement.

In recent years, a variety of interfacial materials for electron transfer have been studied such as metal oxides (ZnO , TiO_2 , etc.), organics ionic salts (CsSt , PFN , etc.) and organic materials (PC_{61}BM , etc.) (Lee et al., 2013; Pathak et al., 2014; Docampo et al., 2013; Li et al., 2018b; 2018c; Huang and Li, 2016; Reinhard et al., 2011; Yang et al., 2012, 2014; Ma et al., 2012; Kuang et al., 2015). Compared to these, metallic stearates are a type of commercially available and cost-effective materials, which consist of an inorganic metallic cation and a long chain aliphatic hydrocarbon radical ion (Li et al., 2014; Wang et al., 2014a,b; Li et al., 2018d). Metallic stearates can be dissolved in the methanol (MeOH) easily to possess good processability. Cesium stearate (CsSt) has been successfully combined with ZnO as interfacial materials in PSCs in our previous work, which resulted in a high PCE with a dramatically enhanced J_{sc} . Additionally, a thin potassium stearate (KSt) film was introduced on the top of ZnO film to passivate its surface defects to fabricate the highly efficient inverted polymer solar cells. Compared to CsSt used for interfacial modification layer of PSCs, potassium ion of KSt has a smaller ionic radius compared to cesium ions so that it is beneficial for ion migration under the external electric field conditions (Wang et al., 2014a,b). In this work, we introduce various stearate salts (Na^+ , K^+ and Cs^+) as interfacial materials to systematically investigate the effects of different ionic radius on the electron transfer of PSCs devices. Interestingly, we found that the key device parameters such as V_{oc} , J_{sc} , fill factor and PCE of polymer solar cells present regular change

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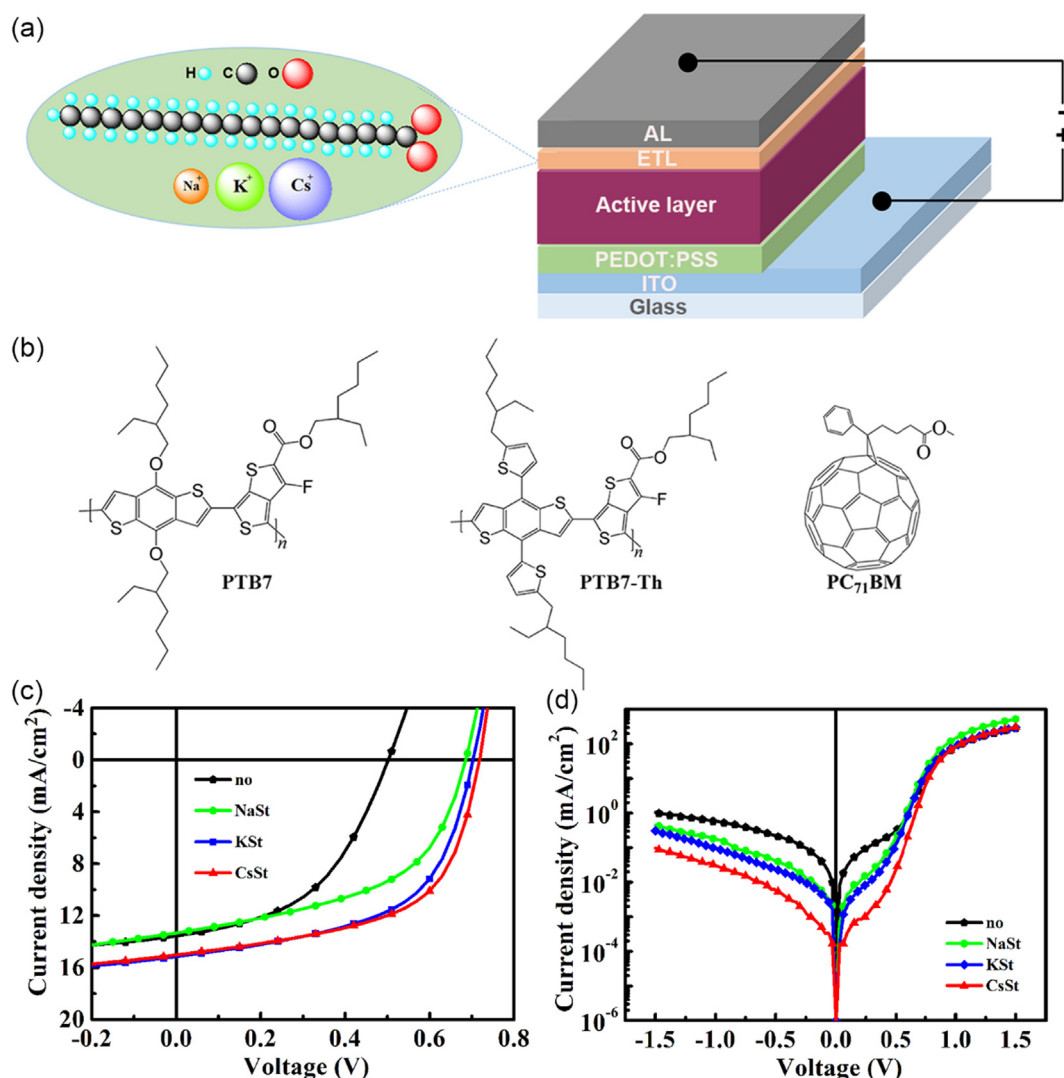


Fig. 1. (a) The device architecture for this study, (b) Chemical structures of the materials used for device fabrication, (c) Illuminated and (d) dark J - V characteristics of ITO/PEDOT:PSS/PTB7:PC₇₁BM/ETL/Al architecture using different cathode interlayers.

with the ionic radius increasing. A series of analysis and measurements such as current density-voltage characteristics, electrochemical and impedance spectroscopy were performed to understand the regularity and the intrinsic reason. The polymer : fullerene active layer that we used comprises [6,6]-phenyl-C₇₁-butyric acid methyl ester (PC₇₁BM) and poly[[4,8-bis[(2-ethylhexyl)oxy]benzo[1,2-b:4,5-b']dithiophene-2,6-diyl][3-fluoro-2-[(2-ethylhexyl)carbonyl]thieno[3,4-b]thiophenedi-yl]] (PTB7) or poly[4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)benzo[1,2-b:4,5-b']di-thiophene-alt-3-fluorothieno[3,4-b]thiophene-2-carboxylate] (PTB7-Th).

2. Experimental details

2.1. Materials

Poly(3,4-ethylenedioxythiophene):polystyrene sulfonate (PEDOT:PSS) was purchased from Clevious, and used as received without further purification. Sodium stearate (NaSt) was purchased from Sinopharm Chemical Reagent Co., Ltd. Cesium stearate (CsSt) was synthesized from stearic acid and cesium carbonate. Potassium stearate (KSt) was purchased from aladdin company. Electron acceptor material PC₇₁BM was commercially available. Electron donor material PTB7 and PTB7-Th was purchased from 1-Material Chemscitech Inc. All these commercially available chemicals were used as received.

2.2. Device fabrication

The device structure was ITO/PEDOT:PSS/PTB7 or PTB7-Th:PC₇₁BM/ETL/Al. The indium tin oxide (ITO) glass substrates were cleaned by sequential ultrasonic treatment in detergent, deionized water, acetone and isopropanol for 15 min respectively, and then blown dry with nitrogen. Subsequently the substrates were treated by UV-ozone treatment for 20 min. The PEDOT:PSS was spin-coated at 4000 rpm on the ITO substrates and then annealed at 140 °C for 15 min. All substrates were transferred to the argon-filled glove box for further processing. Then the active layer was made by spin-coating the active materials in mixed solvent of chlorobenzene/1,8-diiodoctane (97:3 vol %) at 2000 rpm for 120 s on the top of PEDOT:PSS layers. The blend ratio of PTB7 or PTB7-Th:PC₇₁BM was 1:1.5 by weight (25 mg/ml). Next, metallic stearates in methanol solutions with a concentration of 1 mg/mL was spin-coated at 4000 rpm for 1 min on the top of active layers. The device fabrication was completed after thermal evaporation of 100 nm of Al as the cathode under vacuum at a base pressure of about 1×10^{-6} Torr. The device area was 0.06 cm². All devices were fabricated from the same solution under the same condition.

2.3. Device characteristics

The current density-voltage (J - V) characteristics of the photovoltaic

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