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Investigation on polymer solar cells by using calcium as an Electron Transportation Layer

Guilin Liu [a], Ying Guo [b], Huimin Yan [b], Bingjie Zhu [b], Guohua Li [b,c,*]

[a] School of Internet of Things Engineering, Jiangnan University, Wuxi 214122, China
[b] School of Science, Jiangnan University, Wuxi 214122, China
[c] Jiangsu (Suntech) Institute for Photovoltaic Technology, Wuxi 214028, China

HIGHLIGHTS

- Ca–S bonds result the shift of energy level and the improvement of V_{oc} is consistent with XPS images.
- The accumulative error during the thermal evaporation is the main reason of I_{sc} and FF decrease.
- Recombination is explored via quantum tunneling theory and it is consistent with experimental data.

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ABSTRACT

This work investigated the transportation and recombination mechanisms of carriers in organic photovoltaic by using calcium (Ca 10 to 50 nm) as the Electron Transportation Layer (ETL). Compared with the sample without ETL layer, the Fermi Energy Level (E_F) moved at least 0.4 eV towards the Lowest Unoccupied Molecular Orbit (LUMO) of P3HT after Ca was inserted. Ca–S bonds at the interface resulted in the shift of Highest Occupied Molecular Orbit (HOMO) which increased V_{oc} to 0.58 V. Meanwhile, the shift of HOMO and low work function of Ca decreased the recombination possibility (from 1.38% to 0.403%), which resulted in 1% improvement of Fill Factor (FF). The experimental results were coincide with theoretical explanation. Additionally, the existence of accumulative error during the thermal evaporation cannot be neglected. This is the main reason for the decrease of I_{sc} and FF.

1. Introduction

Organic photovoltaic (OPV) [1–4] has been widely investigated due to its low-cost, flexibility, light-weight and potential applications. The performance of OPV has steadily increased to higher levels. The power conversion efficiency (PCE) of OPV up to 10.6% [5] has been achieved, and the stability can be maintained for thousands of hours [6,7]. Research of OPV includes morphology changes [8,9], PCE [7,8], device stability [9,10], processing and manufacturing [10,11]. All of the above have been widely studied. However, the modification of Electron Transportation Layer (ETL) as well as its quantum mechanism [11] was rarely reported. Moreover, leakage current [12,13] in OPVs still needs to be clarified. In this paper, Calcium (Ca) was used as ETL because of its lower electro-negativity [14], higher conductivity [15], and better matching with aluminum (Al) [16].

The aim of this work is to understand the mechanism of Ca as an ETL layer. Additionally, the effect of applied voltage on recombination is also investigated in Bulk HeteroJunction (BHJ) solar cells.

* Corresponding author at: School of Science, Jiangnan University, Wuxi 214122, China.
E-mail address: guohua_li55@yahoo.com (G. Li).

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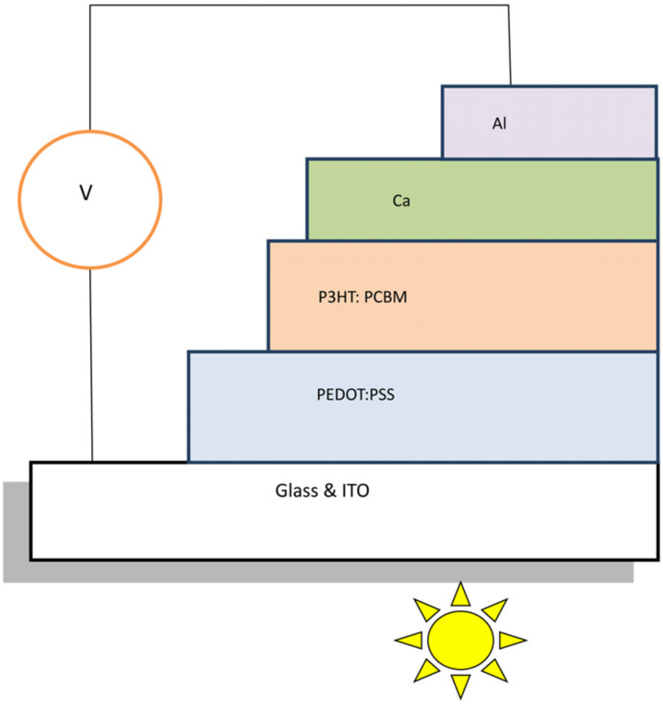

Fig. 1. Layered structure of the polymer solar cell module.

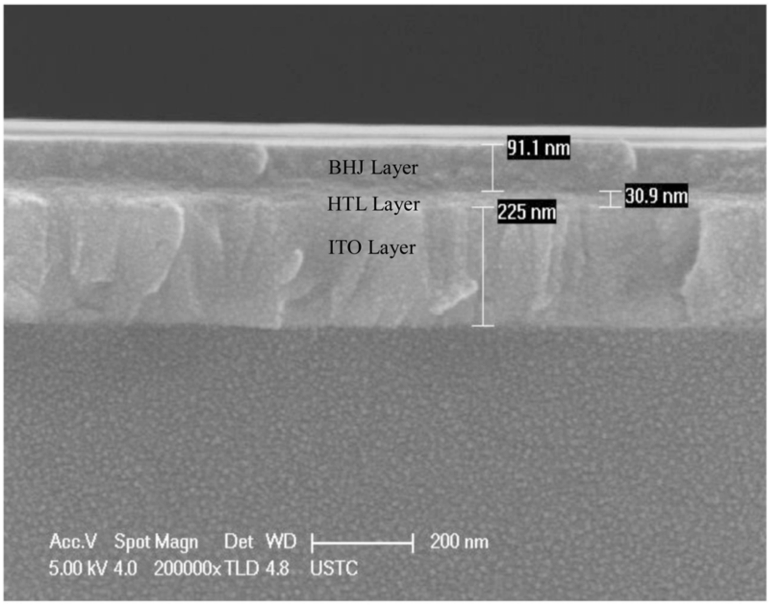

Fig. 2. SEM image of active layer, HTL layer and ITO substrate.

2. Experiments

The OPV samples structure has been illustrated in Fig. 1. Devices were fabricated on pre-cleaned and etched conducting indium tin oxide (ITO) glass (Delta Technologies, $R_S = 7\Omega$ sq^{-1} (Delta Technologies Ltd, Stillwater, Minnesota)) which formed the transparent bottom electrode. The glass substrates were sequentially cleaned by ultrasonic treatment in acetone, isopropyl ethanol, and De-Ionized (DI) water. On the top of the ITO, a layer of p-type poly (3, 4-ethylenedioxythiophene): poly (styrenesulfonate) (PEDOT: PSS, Sigma-Aldrich), used as Hole Transport Layer (HTL) layer, was spin-coated on ITO at 3000 rpm. Then, BHJ layer based on poly (3-hexylthiophene) (P3HT, Sigma-Aldrich) and phenyl C_{61} butyric acid methyl