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Interface modification of organic photovoltaics by combining molybdenum oxide (MoO_x) and molecular template layer

Haichao Duan [a,b], Junliang Yang [a,b,*], Lin Fu [a,b], Jian Xiong [a,b], Bingchu Yang [a,b], Jun Ouyang [a,b], Conghua Zhou [a,b], Han Huang [a,b], Yongli Gao [a,b,c]

[a] Institute of Super-microstructure and Ultrafast Process in Advanced Materials, School of Physics and Electronics, Central South University, Changsha, Hunan 410083, China
[b] Hunan Key Laboratory for Super-microstructure and Ultrafast Process, School of Physics and Electronics, Central South University, Changsha, Hunan 410083, China
[c] Department of Physics and Astronomy, University of Rochester, Rochester, NY 14627, USA

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ABSTRACT

We report discrete heterojunction small molecular organic photovoltaics (OPVs) with enhanced performance by modifying the interface using molybdenum oxide (MoO_x) and molecular template layer perylene-3,4,9,10-tetracarboxylic-3,4,9,10-dianhydride (PTCDA). A large increase in open-circuit voltage was obtained in copper phthalocyanine/fullerene, *i.e.*, CuPc/C_{60} and CuPc/PCBM, discrete planar heterojunction photovoltaics with an insertion of 5 nm MoO_x hole transport layer at the interface between the anode electrode and the CuPc donor layer. It results from the band bending at the interface and the pinning of the highest occupied molecular orbital level of CuPc to the Fermi level of MoO_x due to the defect states (oxygen vacancies) in MoO_x thin films. Moreover, the short-circuit current showed an efficient improvement by inserting a 1 nm PTCDA layer at the interface between the MoO_x layer and the CuPc layer. The PTCDA layer induces the growth of CuPc thin film with lying-down molecular arrangement, supporting the charge transports along the vertical direction. The power conversion efficiencies of CuPc/C_{60} and CuPc/PCBM discrete planar heterojunction photovoltaic devices were improved from about 0.80% to 1.50% with inserting both MoO_x and PTCDA layers. The results suggest that the performance of organic discrete planar heterojunction photovoltaics could be optimized by interface modification with combining hole transport layer and molecular template layer, which are potentially suitable for other highly efficient OPVs, such as small molecular tandem OPVs.

1. Introduction

Organic photovoltaic cells (OPVs) are a promising cost-effective alternative to conventional inorganic electronics for their advantages of light weight, low cost, and flexibility. Significant progress has been achieved in the development of photovoltaic materials and device structures since the report on planar heterojunction OPVs by C. W. Tang [1–5]. Nowadays considerable attention has also been paid to small molecular semiconductor OPVs due to their well-defined molecular structure, definite molecular weight, and high purity without batch to batch variations [6–10]. The interface is of great importance to the performance of OPV devices, and dramatically influences the device parameters, such as short-circuit current (J_{sc}), open-circuit voltage (V_{oc}), and fill factor (*FF*). Through optimizing the interface properties by hole transport layer (HTL) materials, electron transport layer (ETL) materials, or inserting interface materials, the power conversion efficiency (*PCE*) of OPV devices could be improved dramatically [11–14].

Molybdenum oxide (MoO_x) is one of the efficient HTL materials for both polymer and small molecular OPVs [15–21]. It has the advantage of easily controlled deposition by thermal evaporation or solution process with little variation in properties, as well as matching with potential large-area printing or coating fabrication for OPV modules. As an efficient HTL in OPVs, MoO_x can normally improve the V_{oc}, such as in poly(3-hexyl thiophene) (P3HT)/fullerene bulk heterojunction OPVs [15] and phthalocyanine/fullerene planar heterojuncton OPVs [17–19]. Especially, MoO_x can dramatically improve the stability of OPVs as compared with the devices without MoO_x layer [19–21]. However, it looks like that MoO_x have no effects on improving the V_{oc} of copper phthalocyanine (CuPc)-based OPV devices [19]. On the other hand, perylene-3,4,9,10-tetracarboxylic-3,4,9,10-dianhydride (PTCDA) molecular template layer growth was developed to tune the molecular orientation and control the quality of molecular thin films, resulting in an improved performance in organic optoelectronic devices [17, 22–26]. In CuPc/fullerene (C_{60}) planar heterojunction OPVs, the insertion of PTCDA layer as a template layer can largely improve the J_{sc}.

* Corresponding author at: Institute of Super-microstructure and Ultrafast Process in Advanced Materials, School of Physics and Electronics, Central South University, Changsha, Hunan 410083, China. Tel.: +86 731 88660256.
E-mail address: junliang.yang@csu.edu.cn (J. Yang).

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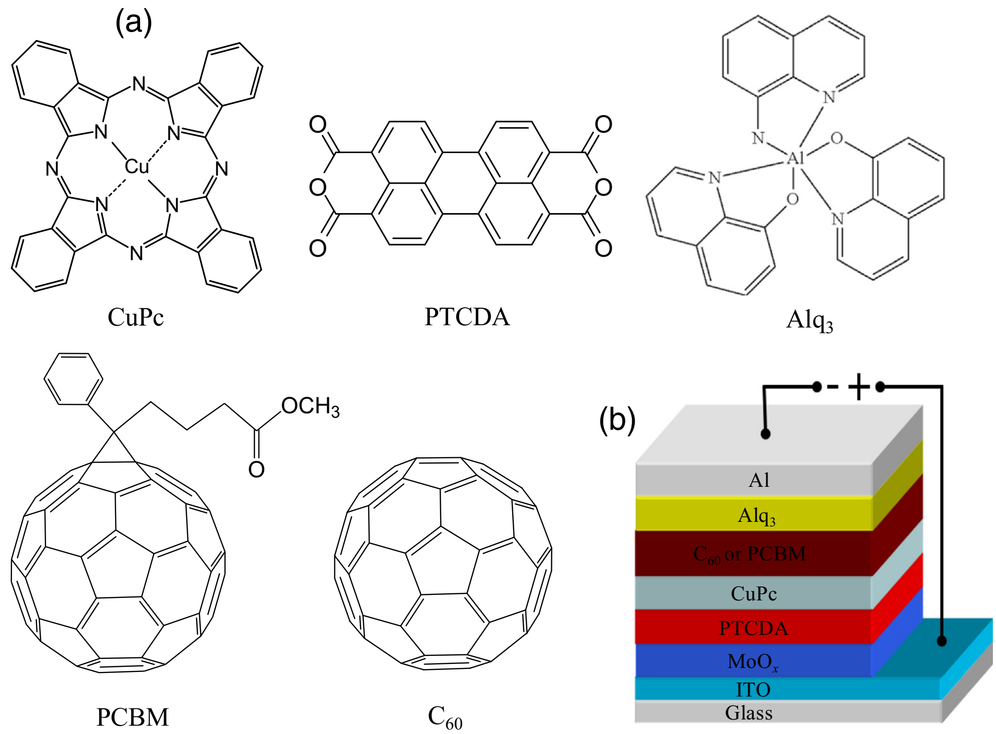

Fig. 1. (a) Molecular structures of CuPc, PTCDA, Alq_3, PCBM and C_{60}. (b) Schematic structure of OPV device with MoO_x and PTCDA layer.

However, the V_{oc} decreases due to the mismatch of energy levels between the PTCDA layer and the indium tin oxide (ITO) electrode [23].

In this research, we combined the MoO_x as an HTL and PTCDA as a molecular template layer between the ITO electrode and the CuPc donor to fabricate small molecular OPVs with the structures of ITO/MoO_x/PTCDA/CuPc/C_{60}/aluminum tris(quinolin-8-olate)(Alq_3)/Al and ITO/MoO_x/PTCDA/CuPc/PCBM/Alq_3/Al. The V_{oc} of CuPc-based OPV devices could be improved, which is different to the report before [19].

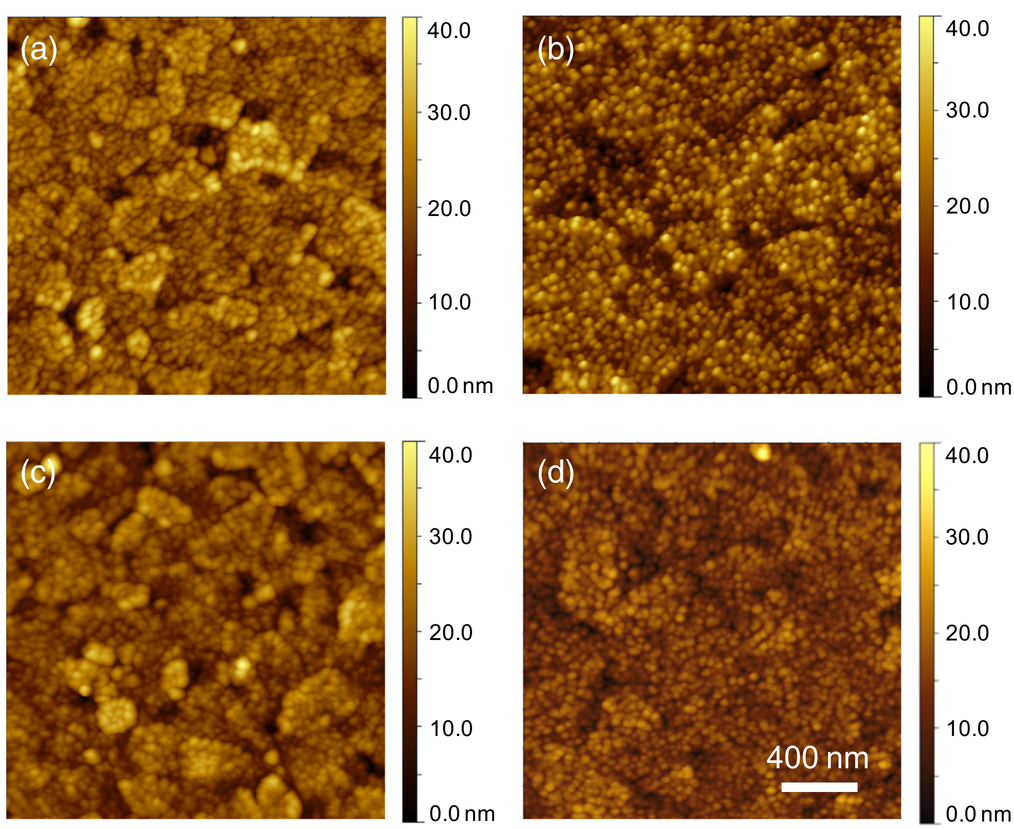

Fig. 2. AFM morphology images with an area of 2 μm × 2 μm (the scale bar is 400 nm for all images.). (a) Glass/ITO (RMS ≈ 4.18 nm), (b) ITO/CuPc (RMS ≈ 4.32 nm), (c) ITO/MoO_x/CuPc (RMS ≈ 4.08 nm), and (d) ITO/MoO_x/PTCDA/CuPC (RMS ≈ 3.94 nm). The thicknesses of CuPC, MoO_x and PTCDA are 40 nm, 5 nm and 1 nm, respectively.