Metal-Doped Copper Indium Disulfide Heterostructure: Environment-Friendly Hole-Transporting Material toward Photovoltaic Application in Organic-Inorganic Perovskite Solar Cell †

Kobra Valadi and Ali Maleki *

Catalysts and Organic Synthesis Research Laboratory, Department of Chemistry, Iran University of Science and Technology, Tehran 16846-13114, Iran; valadi43@gmail.com
* Correspondence: maleki@iust.ac.ir; Tel.: +98-21-73228313; Fax: +98-21-73021584
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Abstract: In this plan, we use Praseodymium metal-doped copper indium disulfide (Pr-doped CIS) heterostructure as hole-transporting materials (HTMs) in the FTO/TiO2/Perovskite absorber/HTM/Au device. And photovoltaic performance of these Pr-doped CIS heterostructure was investigated in the fabrication of the organic-inorganic perovskite solar cells (organic-inorganic PSCs).

Keywords: green electricity; Pr-coated CuInS2 heterostructure; perovskite solar cells; hole-transporting material; solar energy

1. Introduction

Recently, by increasing global warming, reducing fossil fuels and increasing greenhouse gas emissions, the generation of green energy through the development of renewable energy sources to provide the human energy needed is excellent importance [1–3]. Generally, among the various sources of renewable energy, such as solar, wind, natural gas and geothermal, solar energy is the most unique source of green energy in the future due to its abundance, ubiquity, unlimited, eco-friendly, low-cost fabrication, clean and easy access [4].

In organic-inorganic PSCs, the CH3NH3PbI3 active layer is sandwiched between the electron-transport layer (ETL) and hole-transporting layer (HTL). The common HTL and in order to are spiro MeOTAD and TiO2, in sequence, were used. As well as the ETL and HTL systems and play considerable roles in photovoltaic parameters of the PSCs [5].

However, the replacement and or removal of hole-transporting materials (HTMs) in order to improve the system stability and decrease device cost is beneficial [6].

On the other hand, hybrid nanocomposites are defined as heterogeneous systems with organic and inorganic components that have at least one of its components smaller than 100 nanometers. These hybrid materials not only create a new compound but also improve their properties and applications in various fields [7–25].

For these reasons, we present a novel strategy for the organic-inorganic PSCs bested on the Pr-doped CuInS2 heterostructure as HTM to improve the device photovoltaic performance and energy diagram of the organic-inorganic PSC system as shown in Scheme 1.
2. Experimental

2.1. General

All the precursor chemicals were obtained from Alfa Aesar and TCL Chemicals.

2.2. Synthesis of Pr-doped CuInS2 Heterostructure

At first, in a 250 mL three-neck flask, 0.01 mmol of CuCl, 0.01 mmol of InCl3, 2 mmol sulfur, 2 mL of OLA surfactant and the solution containing Pr was added to the reaction system to synthesis of Pr-doped CuInS2 by using an oil bath at 110 °C for 30 min under N2 gas were combined. Next, the formation of a black solution, about 2 h remains at 210 °C temperature. The product mixture was cooled down to ambient temperature. Then, the product was washed three times with cyclohexane. Second, 1 mL of cyclohexane, 1 mL of formamide and 10 mg Na2S·9H2O were mixed and injected into the flask quickly, and the mixture reaction was vigorously by stirred for 10 min. The black solution was centrifuged (12,000 rpm, 15 min for per step) and washed several times with EtOH and H2O. Then, dried in a vacuum oven at 60 °C overnight.

2.3. Device Fabrication of PSCs

F-doped tin oxide (FTO) glasses were washed with distilled water, acetone and ethanol in the ultrasonic bath (10 min for per step), and it was dried under N2 gas. Then, to deposition of TiO2 compact layer, a titanium (IV) isopropoxide (TTIP) solution at 2000 rpm for 30 s was spin-coated onto the FTO substrate and then dried 500 °C. After that, to loaded TiO2 mesoporous layer, TiO2 paste dissolved in EtOH and was spin-coated on the upper TiO2 compact layer.

Perovskite absorber layer was loaded via double step spin-coating method on the electron transporting layer; to deposition of lead iodide layer, a 1 M of PbI2 solution was synthesized by added 462 mg lead iodide powder in DMF aprotic solvent at 80 °C. After than 20 μL of prepared solution was spin coating on the nanostructure substrate for 3000 rpm at 10 s. 200 μL of MAI solution (35 mg MAI precursor in 5 mL isopropanol) was loaded by 2000 rpm for 10 s and was heated at 100 °C for 30 min to form CH3NH3PbI3 absorber compound. The Pr-coated CuInS2 suspension as a HTMs layer was loaded at 4000 rpm for 30 s on the top surface of the FTO/TiO2 compact/TiO2
mesoporous/Perovskite absorber system. Finally, a gold layer was coated via thermal evaporation in the perovskite surface.

3. Results and Discussion

To study, the photoelectric performance of the FTO/TiO₂/perovskite/HTM/Au organic-inorganic PSC based on Pr-doped CIS sample as HTM was tested by current intensity-voltage (J-V) curve and reported under the AM 1.5 G, 100 mW/cm² illumination (Figure 1). For this systems, the open-circuit voltage (V₀), short-circuit current density (Jₛ𝑐) and highest power conversion efficiency (PCE) electrical parameters were summarized and listed in Table 1. Which could be ascribed to the decreases the recombination of electron-hole pairs and very increase contact surface with perovskite films.

![J-V curves of organic-inorganic PSC based on Pr-doped CIS ETLs under AM 1.5 G, 100 mW/cm² illumination.](image)

Figure 1. J-V curves of organic-inorganic PSC based on Pr-doped CIS ETLs under AM 1.5 G, 100 mW/cm² illumination.

| Electron Transporting Layers | J_sc (mA/cm²) | V_OC (V) | FF (%) | Efficiency (%) |
|-----------------------------|--------------|----------|--------|---------------|
| FTO/TiO₂/Perovskite/Pr-doped CIS/Au | 7.22 | 0.76 | 20.03 | 10.99 |

4. Conclusions

In summary, in this study, we have suggested a new Pr-doped CIS as the THM layer and its photoelectric performance tested for organic-inorganic PSC by the J-V curve.

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Conflicts of Interest: The authors declare no conflict of interest.
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