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Author: Hongjie Jia Shuying Cheng Hong Zhang Jinling Yu Yunfeng Lai



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Band alignment at the $\text{Cu}_2\text{SnS}_3/\text{In}_2\text{S}_3$ interface measured by X-ray photoemission spectroscopy

Hongjie Jia^{1,2}, Shuying Cheng^{*1,2}, Hong Zhang^{1,2}, Jinling Yu^{1,2}, Yunfeng Lai^{1,2}

1. College of Physics and Information Engineering, and Institute of Micro-Nano Devices and Solar Cells, Fuzhou University, Fuzhou, 350116, P.R.China
2. Jiangsu Collaborative Innovation Center of Photovoltaic Science and Engineering, Changzhou, 213164, P.R.China

*Corresponding author email: sycheng@fzu.edu.cn

Highlights

- The band alignment at the $\text{Cu}_2\text{SnS}_3/\text{In}_2\text{S}_3$ heterojunction interface has been measured by XPS.
- The valence and conduction band offset were determined to be 1.27 ± 0.10 eV and 0.58 ± 0.10 eV for $\text{Cu}_2\text{SnS}_3/\text{In}_2\text{S}_3$.
- The conduction band offset at the $\text{Cu}_2\text{SnS}_3/\text{In}_2\text{S}_3$ heterojunction has a spike-like behavior and the interface is a 'type I'.
- The conduction band offset of 0.58 eV is too high to inject electron from Cu_2SnS_3 layer to In_2S_3 layer.

Abstract: This paper focused on investigating the band alignment at the Cu_2SnS_3 (CTS)/ In_2S_3 heterojunction interface by X-ray photoemission spectroscopy. An In_2S_3 over-layer was grown on a CTS thin film, which was grown by sulfurization of vacuum thermal evaporated Sn-Cu metallic precursors in a $\text{H}_2\text{S}:\text{N}_2$ atmosphere. The valence band offset (VBO) at the CTS/ In_2S_3 interface was measured to be 1.27 ± 0.10 eV. The conduction band offset (CBO) was calculated from the measured VBO, giving (0.58 ± 0.10) eV. These values show that the CBO has a spike-like behavior and the interface is a 'type I'.

Keywords: Band Alignment; Cu_2SnS_3 / In_2S_3 Heterojunction; Conduction Band Offset; XPS

1. Introduction

Cu_2SnS_3 (CTS) is considered a promising candidate for thin film solar cells absorber material because it has good characteristics such as high optical absorption coefficient ($>10^4\text{cm}^{-1}$) [1-3], suitable direct band gap of ~ 1.3 eV (tetragonal structure) or ~ 0.9 eV (cubic structure)[4], high theoretical light conversion efficiency (above 33%) [5], abundant and non-toxic elements. Therefore, there were lots of reports on CTS thin film solar cells by several research groups using different approaches, including sputtering [2, 6, 7], evaporation [8, 9], successive ionic layer adsorption and reaction (SILAR)[10], electrodeposition [11], solid reactions [3, 12, 13], spray pyrolysis [14], and solvothermal synthesis [15]. However, it is quite difficult to obtain CTS thin film solar cells with high conversion efficiencies by experiments. At present, the highest conversion efficiency of the CTS solar cell reported is 2.92% [8, 9, 11, 16-19]. The prevalent low efficiencies can be attributed to various sources, such as bulk material impurities and defects,

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