IOP Publishing J. Phys. Energy 5 (2023) 045007 https://doi.org/10.1088/2515-7655/acf688

Journal of Physics: Energy

CrossMark

RECEIVED
2 May 2023

REVISED
7 August 2023

ACCEPTED FOR PUBLICATION
4 September 2023

PUBLISHED
14 September 2023

PAPER

Design of n-i-p and p-i-n Sb_2Se_3 solar cells: role of band alignment

Marwa S Salem[1,2], Mohamed Okil[3], Ahmed Shaker[4,*], Abdullah Albaker[5] and Mansoor Alturki[5]

[1] Department of Computer Engineering, College of Computer Science and Engineering, University of Ha'il, Ha'il 55211, Saudi Arabia
[2] Department of Electrical Communication and Electronics Systems Engineering, Faculty of Engineering, Modern Science and Arts University (MSA), Cairo 12556, Egypt
[3] Department of Basic Engineering Sciences, Benha Faculty of Engineering, Benha University, Benha 13512, Egypt
[4] Department of Engineering Physics and Mathematics, Faculty of Engineering, Ain Shams University, Cairo 11535, Egypt
[5] Department of Electrical Engineering, College of Engineering, University of Ha'il, Ha'il 81451, Saudi Arabia
[*] Author to whom any correspondence should be addressed.

E-mail: ahmed.shaker@eng.asu.edu.eg

Keywords: Sb_2Se_3, ETL, HTL, band alignment, CBO, VBO, PCE

Supplementary material for this article is available online

Abstract

Investigations into novel device architectures and interfaces that enhance charge transport and collection are necessary to increase the power conversion efficiency (PCE) of antimony selenide (Sb_2Se_3) solar cells, which have shown great promise as a low-cost and high-efficiency alternative to conventional silicon-based solar cells. The current work uses device simulations to design p-i-n and n-i-p Sb_2Se_3-based solar cell structures. The n-i-p configuration is investigated by comparing distinct electron transport layer (ETL) materials to get the best performance. While certain ETL materials may yield higher efficiencies, the *J–V* curve may exhibit S-shaped behavior if there is a misalignment of the bands at the ETL/absorber interface. To address this issue, a proposed double ETL structure is introduced to achieve proper band alignment and conduction band offset for electron transport. A PCE of 20.15% was achieved utilizing (ZnO/ZnSe) as a double ETL and Spiro-OMeTAD as a hole transport layer (HTL). Further, the p-i-n configuration is designed by proposing a double HTL structure to facilitate hole transport and achieve a proper valence band offset. A double HTL consisting of (CuI/CuSCN) is used in conjunction with ETL-free configuration to achieve a PCE of 21.72%. The simulation study is conducted using the SCAPS-1D device simulator and is validated versus a previously fabricated cell based on the configuration FTO/CdS/Sb_2Se_3/Spiro-OMeTAD/Au.

1. Introduction

Solar cells are a key renewable energy resource that has gained significant attention in recent years due to their potential to address the challenges of climate change, energy security, and sustainability. The energy generated by solar cells is free, abundant, and widely available, making them an ideal solution for meeting the growing electricity demand. In recent years, photovoltaic (PV) technology has advanced rapidly, resulting in increased efficiency, reduced costs, and improved reliability [1, 2]. Silicon solar cells are the most commonly employed and mature PV technology, accounting for more than 90% of the global market [3]. Silicon solar cells have several advantages, including high efficiency, long lifespan, and low maintenance requirements. They are also environmentally friendly [4]. In recent years, research has focused on improving silicon solar cells' efficiency through advanced manufacturing techniques, such as passivation and surface texturing, as well as the incorporation of new structures [3–5]. Alternatively, thin film solar cells (TFSCs) are a type of PV technology that uses thin layers of semiconductor materials [6]. Unlike traditional silicon solar cells, TFSCs are flexible, lightweight, and can be produced at lower costs, making them an attractive option for many applications. TFSCs use less material than traditional silicon solar cells, making them cheaper to produce. They can also be produced using roll-to-roll manufacturing techniques, allowing for high-volume and