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Design and analysis of Perovskite/Sb_2Se_3 systems: Towards efficient 2-T HTL-free tandem solar cells

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ABSTRACT

This paper investigates the potential of perovskite and Sb_2Se_3 as front and bottom absorber materials, respectively, for two-terminal tandem solar cells (TSCs), focusing on optimizing design and enhancing performance. The study begins by evaluating the standalone sub-cells, calibrating them against experimental data to establish a reliable baseline. We then examine a fabricated four-terminal perovskite/Sb_2Se_3 TSC to explore and compare its foundational characteristics. Moving forward, we concentrate on optimizing a 2-T tandem structure, particularly emphasizing the development of a hole-transporting layer (HTL)-free design. This approach aims to address fabrication challenges related to the instability and degradation of organic HTLs typically used in such systems. The 2-T HTL-free tandem device with optimizing thickness of both absorber layers showed a power conversion efficiency (*PCE*) of 16.96 %. Following the proposed 2-T HTL-free tandem design, the variation of the conduction band offset (CBO) at the electron-transporting layer (ETL)/absorber interfaces and the doping concentration of the ETLs is investigated to evaluate the corresponding effects. A *PCE* of 23.08 % is obtained upon optimizing the CBO and doping levels of both ETLs. Additionally, we examined the influence of modifying the bandgap of the front perovskite absorber layer ($E_{g,Top}$), which is vital for achieving balanced spectral absorption and improving overall efficiency. Furthermore, we conducted an in-depth analysis of the influence of different absorber layer thicknesses, aiming to optimize light absorption and realize current matching between both sub-cells. At the designed matching current density, the optimum efficiency is accomplished, giving J_{SC}=17.55 mA/cm^2, and *PCE*=25.69 % for $E_{g,Top}$ = 1.7 eV. Utilizing Silvaco Atlas device simulator package, simulations are performed under standard AM1.5G illumination conditions. Our findings demonstrate the feasibility and potential benefits of a 2-T HTL-free tandem configuration, paving the path for more efficient and stable perovskite/Sb_2Se_3 TSCs.

1. Introduction

Solar cells represent a crucial technology in the pursuit of renewable energy, as they offer a sustainable power source [1]. Among the distinct categories of solar cells, single-junction solar devices are the most widely employed and researched. Silicon-based cells are remarkably the most common type of single-junction cells, dominating the market due to their well-established technology, stable performance, and abundance of raw materials [2]. In recent years, various approaches have been researched to push the efficiency and/or decrease the manufacturing cost of Si-based photovoltaic cells, such as refining light absorption through surface texturing and anti-reflective coatings and incorporating advanced cell architectures like passivated emitter and rear cell, microstructure and nanowire designs [3–9]. However, despite these advancements, Si-based solar cells face inherent efficiency limitations. The calculated theoretical maximum power efficiency for a single-junction Si PV cell, known as Shockley-Queisser limit, is around 33 % [10]. Practical efficiencies achieved in commercial Si solar cells are generally lower, often less than 27 % [11]. While recent technological innovations can lead to marginal efficiency gains, they often come with

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