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PAPER

Optimization of all-polymer/Sb_2Se_3 tandem solar cells for enhanced efficiency: a comprehensive TCAD modeling approach

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Abstract

This paper introduces a novel tandem configuration, utilizing an all-thin film all-polymer solar cell (all-PSC) with a wide bandgap of 1.76 eV for the front cell and Sb_2Se_3 with a narrow bandgap of 1.2 eV for the bottom cell. The design of this tandem is performed by comprehensive optoelectronic TCAD tools, essential for optimizing parameters across multiple layers to reach maximum power conversion efficiency (*PCE*). Experimental validation of models is conducted through calibration and validation against fabricated reference all-polymer and Sb_2Se_3 solar cells, yielding calibrated PCEs of approximately 10.1% and 10.5%, respectively. Subsequently, validated simulation models for both top and rear cells are utilized to design a 2-T all-polymer/Sb_2Se_3 tandem cell, which initially achieves a *PCE* of 10.91%. Through systematic optimization steps, including interface engineering and homojunction structure design, a remarkable PCE of 24.24% is achieved at the current matching point, showcasing the potential of our proposed tandem solar cell design. This study represents a significant advancement in the field of thin-film tandem solar cells, offering promising avenues for efficient and cost-effective photovoltaic technologies, particularly in applications requiring flexibility.

1. Introduction

Currently, the energy demand is rapidly increasing, and clean energy sources, notably solar cells, offer promising solutions. Solar energy has emerged as a highly efficient alternative to traditional energy resources. Si solar cells lead the photovoltaic (PV) market, constituting 90% of the industry, with efficiencies exceeding 25% [1–3]. Nonetheless, despite their remarkable performance, Si cells encounter inherent limitations in photon absorption, dictated by the limited range of wavelengths they can effectively capture, due to their material's energy gap, and carrier thermalization losses. Moreover, the efficiencies of Si-based and thin-film technologies, such as CIGS and CdTe, have begun to reach saturation levels, hovering around 26% and 23%, respectively [4]. Tandem (multi-junction) PV systems have emerged as a solution to alleviate these limitations, utilizing sub-cells with different complementary bandgaps to absorb various wavelengths of sunlight. In this regard, a two-junction tandem design has shown theoretical potential, with a front PV cell having a bandgap of 1.7 eV and a rear solar cell having a bandgap of 1.12 eV, achieving a notable efficiency of up to 40% [5]. Various tandems have been experimentally and theoretically explored in the literature, featuring both 2-T and 4-T configurations. These include perovskite/Si [6, 7], Sb_2S_3/Si [8], perovskite/perovskite [9], perovskite/CIGS [10, 11], perovskite/organic [12, 13], and many other tandems incorporating diverse material systems.

Recent advancements have been witnessed in all-polymer solar cells (all-PSCs) utilizing polymerized small molecular acceptors (PSMAs). These all-PSCs, featuring bulk heterojunction (BHJ) photoactive layers comprising a *p*-type conjugated polymer donor and an *n*-type conjugated polymer acceptor, have garnered rising interest [14]. This interest is owed to their superior mechanical properties, thermal stability, photostability, and environmentally friendly solar energy conversion [15]. An exemplary achievement was