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# Advancements in eco-friendly lead-free perovskite/$Sb_2Se_3$ tandem solar cells: TCAD simulations

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ABSTRACT

In light of the urgent need for sustainable energy solutions, this research addresses the critical environmental concerns of traditional lead-based perovskite materials. This paper explores advancements in an eco-friendly tandem solar cell (TSC) that incorporates both lead-free wide bandgap perovskite and narrow bandgap antimony selenide ($Sb_2Se_3$), focusing on optimization strategies utilizing TCAD numerical simulations. The study begins with the calibration of experimental standalone solar cells based on wide bandgap lead-free perovskite (1.62 eV) with a *p-i-n* heterostructure and narrow bandgap $Sb_2Se_3$ (1.2 eV) with an *n-i-p* configuration. The research then transitions to evaluating the lead-free perovskite/$Sb_2Se_3$ system in a four-terminal (4-T) tandem, followed by optimization of the top cell to an *n-i-p* heterostructure for compatibility with a two-terminal (2-T) structure. Key optimization areas include replacing the organic hole transport layer (HTL) with other inorganic candidates, conduction band offsets (CBOs), and absorber thicknesses. Through these optimizations, the 2-T tandem design achieves a significant improvement, with a simulated *PCE* reaching 30.96 %. Numerical simulations using TCAD tools are employed to predict performance and guide experimental modifications. This research integrates material science and advanced TCAD simulations to optimize TSC performance with a focus on eco-friendly materials for environmental sustainability.

## 1. Introduction

The growing importance of renewable energy, including solar energy, is underscored by recent advancements in sustainable technologies and self-sustaining energy systems that enhance energy resilience, improve efficiency, and promote eco-friendly solutions [1–3]. Reducing the environmental impact of energy production is crucial, with sustainable materials and an efficient design in solar energy helping to lower ecological footprints and support cleaner power sources [4,5]. Traditional silicon-based solar cells dominate the photovoltaic sector thanks to their established technology and relatively high efficiency. Presently, commercially produced Si solar modules achieve efficiencies ranging from 16 % to 22 % [6]. Despite their dominance, Si solar cells face constraints such as high manufacturing costs and diminishing returns in efficiency improvements [7]. Researchers actively explore alternative materials and technologies to reduce costs and enhance performance. In this regard, thin film technology has emerged as a noteworthy advancement in photovoltaic (PV) systems, offering a range of benefits over traditional silicon-based solar cells [8]. This technology engages the deposition of thin layers of PV materials onto a substrate, creating flexible, lightweight, and cost-effective solar panels. The key to thin film technology's success lies in its ability to leverage diverse materials as well as manufacturing processes to optimize performance and reduce production costs. Key types include CdTe, known for high efficiency and low cost despite environmental concerns; CIGS which offers high flexibility and efficiency but involves complex production; and a-Si which is inexpensive and flexible but has lower efficiency [9]. Recent studies on stability, environmental implications, and optimal design of sustainable PV systems highlight the critical role of environmentally friendly materials and hybrid energy solutions in enhancing reliability and reducing emissions in grid-connected applications [10–12]. Among the advancements in PV technology, lead-free perovskite and $Sb_2Se_3$ solar cells stand out as particularly noteworthy for their eco-friendly and low-cost processing attributes.

Perovskite materials have revolutionized the field of solar energy with their excellent light absorption capabilities and efficient charge transport properties. Recent advancements in lead-based PSCs have

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