



## Full Length Article

## Full optoelectronic simulation of all antimony chalcogenide thin film tandem solar cell: Design routes from 4-T to 2-T configuration



Marwa S. Salem<sup>a,b</sup>, Ahmed Shaker<sup>c,\*</sup>, Chao Chen<sup>d</sup>, Luying Li<sup>d</sup>, Mohamed Abouelatta<sup>e</sup>,  
Arwa N. Aledaily<sup>f</sup>, Walid Zein<sup>c</sup>, Mohamed Okil<sup>g</sup>

<sup>a</sup> Department of Computer Engineering, College of Computer Science and Engineering, University of Ha'il, Ha'il, Saudi Arabia

<sup>b</sup> Department of Electrical Communication and Electronics Systems Engineering, Faculty of Engineering, Modern Science and Arts University (MSA), Cairo, Egypt

<sup>c</sup> Department of Engineering Physics and Mathematics, Faculty of Engineering, Ain Shams University, Cairo, Egypt

<sup>d</sup> Wuhan National Laboratory for Optoelectronics (WNLO) and School of Optical and Electronic Information, Huazhong University of Science and Technology (HUST), Wuhan, China

<sup>e</sup> Department of Electronics and Communications, Faculty of Engineering, Ain Shams University, Cairo, Egypt

<sup>f</sup> Department of Computer Science and Information, College of Computer Science and Engineering, University of Ha'il, Ha'il, Saudi Arabia

<sup>g</sup> Department of Basic Engineering Sciences, Benha Faculty of Engineering, Benha University, Benha, Egypt

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## ABSTRACT

Antimony chalcogenide, as a newcomer to light harvesting materials, is regarded as an auspicious contender for incorporation as a photoactive layer in thin film tandem solar cells (TFTSCs). The current study introduces the design of all-antimony chalcogenide TFTSC comprised of an Sb<sub>2</sub>S<sub>3</sub> (1.7 eV) front subcell and an Sb<sub>2</sub>Se<sub>3</sub> (1.2 eV) rear subcell. The challenges to migrating from four-terminal (4-T) to two-terminal (2-T) designs are highlighted and possible solutions are proposed. To commence, a calibration procedure for the two subcells is conducted in alignment with experimental investigations. The benchmarked solar cells yield a power conversion efficiency (PCE) of 8.08 % for the upper subcell and 10.58 % for the lower subcell. Subsequently, upon integration of both subcells within the initial 4-T Sb<sub>2</sub>S<sub>3</sub>/Sb<sub>2</sub>Se<sub>3</sub> TFTSC, the resultant PV cell attains a PCE of 12.27 %. Before transitioning it to a more efficient 2T tandem configuration, we explore alternative inorganic HTL materials to the Spiro-OMeTAD HTL to overcome its practical considerations. Cu<sub>2</sub>O is found to be the best HTL alternative to be included for both subcells. Upon stacking into the tandem structure, the combined cell exhibited an efficiency of 15.68 % and a notable  $J_{sc}$  of 16.23 mA/cm<sup>2</sup>. To further enhance the tandem performance, the device structure is optimized by engineering the CBO of two sub-cells and employing a double ETL design for the front sub-cell. At the considered current matching criterion, the tandem device PCE and  $J_{sc}$  are boosted to 27.86 % and 17.60 mA/cm<sup>2</sup>, respectively. Based on this full optoelectronic analysis, developed in the Silvaco TCAD environment, a 2-T all antimony chalcogenide tandem configuration can be realized and optimized, paving the way for future experimental endeavors.

## 1. Introduction

The widespread adoption of Si solar cells has propelled photovoltaic (PV) technology by offering efficient energy conversion [1]. To push Si solar cells further, some novel structures were proposed, including microstructures [2], and nanowires [3]. Additionally, it was shown that the insertion of multiple quantum wells made of Si<sub>0.95</sub>Ge<sub>0.05</sub> improves the efficiency by a factor of 1.37 compared to that obtained for conventional Si nanowires [4]. Other studies related to III-V materials solar cells also show advancements, including proposed quantum dot GaAs/GaAsP

structures [5]. Nonetheless, thin film solar cells have arisen as a favorable choice, boasting advantages such as flexibility, lightweight design, and cost-effectiveness, setting them apart from their Si and III-V counterparts.

Tandem solar cells, representing a remarkable advancement in PV systems, harness the cumulative power of multiple solar cell layers to capture a broader spectrum of sunlight [6–8]. This tandem approach significantly enhances the overall PCE as compared to single-junction PV cells. In the context of tandem cells, antimony selenide (Sb<sub>2</sub>Se<sub>3</sub>) and antimony sulfide (Sb<sub>2</sub>S<sub>3</sub>) materials hold immense prospects as

\* Corresponding author.

E-mail address: [ahmed.shaker@eng.asu.edu.eg](mailto:ahmed.shaker@eng.asu.edu.eg) (A. Shaker).

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