

**NUMERICAL SIMULATION OF BiSI AND BiSeI
ABSORBER MATERIAL FOR PEROVSKITE BASED
SOLAR CELLS USING SCAPS 1-D**

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Thesis submitted in partial fulfillment of the requirement for the degree
Master of Science in Material Science

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April 2024

Declaration and the Statement of the Supervisor

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I declare that this is my own work and this thesis/dissertation does not incorporate without acknowledgement any material previously submitted for a Degree or Diploma in any other University or Institute of higher learning and to the best of my knowledge and belief it does not contain any material previously published or written by another person except where the acknowledgement is made in the text. I retain the right to use this content in whole or part in future works (such as articles or books).

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Abstract

The research is centered on numerically simulating lead-free bismuth Chalcogenide Solar Cells based on thin films of Bismuth Sulfur Iodide (BiSI) and Bismuth Selenium Iodide (BiSeI) through the Solar Cell Capacitance Simulator (SCAPS 1D). The cell architecture comprising with the titanium dioxide (TiO_2) for the electron transport layer (ETM) and the Spiro-OMeTAD for the hole transport layer (HTM). Furthermore, we employed Bismuth Sulfur Iodide (BiSI) and Bismuth Selenium Iodide (BiSeI) as the absorbing layers, sandwiched between two electrode materials. Specifically, Fluorine-doped tin dioxide (FTO) served as the front electrode contact, and Gold (Au) was utilized as the back electrode contact.

During the research, the simulations were conducted using the SCAPS simulator to investigate the performances of the cell by varying thickness of the absorbing layer and the operating temperature. This straightforward cell architecture facilitated a comprehensive exploration of device parameters. The maximum power conversion efficiency (PCE) of 16.19% (open-circuit voltage V_{oc} of 1.0066 V, short-circuit current J_{sc} of 28.255 mA/cm^2 , and fill factor FF of 56.37%) is obtained at 1500 nm BiSI layer thickness for an optimized device with TiO_2 as the ETL and Spiro-OMeTAD as the HTL for both materials. The maximum power conversion efficiency (PCE) of 22.59 % (open-circuit voltage V_{oc} of 1.1819 V, short-circuit current J_{sc} of 31.989 mA/cm^2 , and fill factor FF of 59.15 %) is obtained at 1500 nm BiSI layer thickness for an optimized device with TiO_2 as the ETL and Spiro-OMeTAD as the HTL for both materials of Bismuth Sulfur Iodide (BiSI) and Bismuth Selenium Iodide (BiSeI), and the optimized device temperature range was determined to be between 290K and 310K while determining 1500 nm as the optimum thickness of the absorbing layer.

Acknowledgement

I would like to express my sincere gratitude to Professor A.S. Galhenage, my project supervisor, for her invaluable guidance, unwavering support, and assistance throughout the project's duration. Her expertise and dedication greatly contributed to the successful completion of this endeavor.

I am also indebted to Professor Marc Burgelman and his team at the University of Gent, Belgium, for their pioneering work in developing and providing the SCAPS 1D software, which was instrumental in conducting the studies for this project. Also, I would be grateful to Mr. U.K.D.M Akamal and Mrs. Sanjeevani Thakshila on helping me to familiar with the SCAPS 1D software and guiding me to find the material data.

Furthermore, I extend my appreciation to all the instructors, with a special mention of Mr. V. Sivahar, the head of the Department, for their expert guidance, insightful recommendations, and unwavering support. I am also grateful to the entire staff of the Department of Materials Science and Engineering at the University of Moratuwa for their role as the primary source of resources that facilitated the successful completion of this project. Their assistance in evaluating and grading the project work was invaluable.

This project would not have been possible without the collective efforts and support of these individuals and institutions, and for that, I am truly thankful.