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

W.A.A.S. Wickramaarachchi (179455J)

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Department of Materials Science and Engineering Faculty of Engineering

University of Moratuwa Sri Lanka

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Declaration and the Statement of the Supervisor

Declaration:

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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The above candidate has carried out research for the Masters thesis under my supervision. I confirm that the declaration made above by the student is true and correct.

Name of the supervisor: Prof. (Mrs.) G.A. Sewvandi

Signature of the supervisor: Date: April 2024

CONTENT

LIST OF FIGURES

LIST OF TABLES

Abstract

The research is centered on numerically simulating lead-free bismuth Chalcohalide 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 Voc of 1.0066 V, short-circuit current Jsc 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 Voc of 1.1819 V, short-circuit current Jsc 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.

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