Numerical Simulation of BiSI and BiSeI Absorber Materials Based Solar Cells

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Recent advancements in perovskite solar cells have improved their stability and addressed toxicity concerns, making them more commercially viable. These cells not only have a less energy-intensive manufacturing process but can also be lead-free, aligning with environmental sustainability goals. The research is centered on numerically simulating lead-free bismuth chalcohalides 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, Bismuth Sulfur Iodide (BiSI) and Bismuth Selenium Iodide (BiSeI) were used 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.

This study investigated the performances of the cell by varying thickness of the absorbing layer and the operating temperature. The maximum power conversion efficiency (PCE) of 16.19% (Voc of 1.01 V, rent Jsc of 28 mA/cm^2, and FF of 56.37%) is obtained at 1500 nm BiSI layer thickness for an optimized device. The maximum PCE of 22.59 % (Voc of 1.18 V, Jsc of 32 mA/cm^2, and FF of 59.15 %) is obtained at 1500 nm BiSeI layer thickness for an optimized device, 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.

The results showed that BiSeI demonstrated superior photovoltaic characteristics at an optimum thickness of 1.5µm compared to BiSI. However, both materials exhibited a significant decrease in performance as the temperature of the photovoltaic cell increased. However, 290K to 310K can be considered as the optimized device temperature range as only slight loss of performance of the material can be observed in the same region of temperature.

Keywords: Fossil fuel, Band gap, Direct band structure, Conversion efficiency, Chalcohalides, Perovskite.