

Numerical Simulation of Lead-free Bismuth Chalcohalide based Perovskite Solar Cells

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Abstract:

Despite the remarkable advances and Power Conversion Efficiency (PCE) accomplished by perovskite solar cells (PSCs), they have been unable to catch the commercial market due to the toxicity caused by lead. Therefore, researchers are exploring sustainable solar cells called non-toxic lead-free PSCs. This research focuses on numerically simulating lead-free Bismuth Chalcohalide, namely, Bismuth Sulfur Iodide (BiSI) and Bismuth Selenium Iodide (BiSel) based Solar Cells through Solar Cell Capacitance Simulator (SCAPS 1D). The cell architecture comprises titanium dioxide as the electron transport layer (ETM) and Spiro-OMeTAD as the hole transport layer (HTM). BiSI and BiSel were employed as absorbing layers. Fluorine-doped tin dioxide and Gold were applied as front and back electrodes respectively. The performance was analyzed by varying absorbing layer thickness. The maximum PCE of 16.19% (open-circuit voltage V_{oc} of 1.01 V, short-circuit current J_{sc} of 28.26 mA/cm², fill factor FF of 56.37%) is achieved at 1500 nm BiSI layer thickness. Correspondingly, a maximum PCE of 22.59% (Voc of 1.18 V, J_{sc} of 31.99 mA/cm², FF of 59.15%) is obtained at 1500 nm BiSel layer thickness. These results highlight the effectiveness of this cell configuration in enhancing the efficiency of lead-free Bismuth Chalcohalide Solar Cells with BiSI and BiSel.

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