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DFT and SCAPS Analysis of an Efficient Lead-Free Inorganic $CsSnI_3$ Based Perovskite Solar Cell by Modification of Hole Transporting Layer

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Abstract : With an abrupt rise in the power conservation efficiency (PCE) of perovskite solar cells (PSCs) within a short span of time, the toxicity of lead was raised as a major hurdle in the path toward their commercialization. In the present research, a systematic investigation of the electrical and optical characteristics of the all-inorganic $CsSnI_3$ perovskite absorber layer was performed with the Vienna Ab Initio Simulation Package (VASP) using the projector-augmented wave method. The presence of inorganic halide perovskite offers the advantages of enhancing the degradation resistance of the device, reducing the cost of cells, and minimizing the recombination of generated carriers. The simulated standard device using a 1D simulator like solar cell capacitance simulator (SCAPS) version 3308 involves FTO/n-TiO_2/$CsSnI_3$ Perovskite absorber/Spiro OmeTAD HTL/Au contact layer. The variation in the device design key parameters such as the thickness and defect density of perovskite absorber, hole transport layer and electron transport layer and interfacial defects are examined with their impact on the photovoltaic characteristic parameters. The effect of an increase in operating temperature from 300 K to 400 K on the performance of CsSnI3-based perovskite devices is also investigated. The optimized standard device at room temperature shows the highest PCE of 25.18 % with FF of 75.71 %, Voc of 0.96 V, and Jsc of 34.67 mA/cm^2. The outcomes and interpretation of different inorganic Cu-based HTLs presence, such as CuSCN, Cu_2O, CuO, CuI, $SrCu_2O_2$, and $CuSbS_2$, here represent a critical avenue for the possibility of fabricating high PCE perovskite devices made of stable, low-cost, efficient, safe, and eco-friendly all-inorganic materials like $CsSnI_3$ perovskite light absorber.

Keywords : $CsSnI_3$, hole transporting layer (HTL), lead-free perovskite solar cell, SCAPS-1D software
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