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Optimization and Numerical Simulation of $Cs_2AgSbBr_6$-Based Lead-Free Perovskite Solar Cells Using SCAPS-1D

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Extensive research into lead-free alternatives has been prompted by the toxicological and environmental issues around lead-based perovskite solar cells. The halide double perovskite $Cs_2AgSbBr_4$ has become a potential absorber material because of its non-toxic composition, good optoelectronic capabilities, and chemical durability [1].

Using the SCAPS-1D platform [2] and the device architecture FTO/ETL/$Cs_2AgSbBr_4$/HTL/Au, this work provides a thorough numerical modeling and optimization of $Cs_2AgSbBr_6$-based solar cells. To determine the ideal charge transport configuration, electron transport layers (TiO_2, SnO_2, ZnO, PCBM) and hole transport layers (Spiro-OMeTAD, CuSCN, NiO, MoO_3) are systematically screened to identify the optimal charge transport arrangement. Crucial elements influencing device performance such as absorber layer thickness, defect density, and doping concentration are investigated through parametric optimization. The results reveal that the optimal ETL/HTL combination significantly enhances power conversion efficiency, offering a viable pathway toward high-performance, environmentally friendly perovskite solar cells.

Fig. 1. Device structure of the $Cs_2AgSbBr_6$-based perovskite solar cell.

Keywords: Lead-free perovskite; Cs2AgSbBr6; SCAPS-1D simulation; Double perovskite solar cell; Electron transport layer

Reference:

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