Title: Revealing the high-performance of a novel Ge-Sn-Based perovskite solar cell by employing SCAPS-1D.

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Abstract: In this study, a novel Ge-Sn based perovskite solar cell (PSC) with the structure FTO/WS_2/ $FA_{0.75}MA_{0.25}Sn_{0.95}Ge_{0.05}I_3$/$MoO_3$/Ag has been designed and thoroughly analyzed employing SCAPS-1D. Drawing attention from the work of Ito *et al* where a similar perovskite-based PSC displayed a poor performance of ~ 4.48% PCE, in which a large conduction band offset (CBO) acts as a critical factor contributing to interfacial recombination and device deterioration. To address this issue, we presented WS_2 as an electron transport layer (ETL) along with MoO_3 as a hole transport layer (HTL), both possessing compatible CBO and valence band offset (VBO) with perovskite material. Through systematic simulations and optimizations, remarkable improvements in the PSC's performance have been acquired, getting a power conversion efficiency (PCE) of 18.97%. The optimized structure involved a 50 nm MoO_3 HTL, 350 nm $FA0.75MA_{0.25}Sn_{0.95}Ge_{0.05}I_3$ light-harvesting layer (LHL), and a 50 nm WS_2 ETL. Bulk defect densities for the LHL and ETL were optimized to 1×10^{15} cm^{-3} and 1×10^{18} cm^{-3}, respectively, significantly superior values than that of reported value in the literature. Particularly, the tolerable defect density of ETL has increased 1000 times more than the published literature. The interfacial tolerable trap density for MoO_3/perovskite increased from 1×10^{14} cm^{-2} to 1×10^{16} cm^{-2}. The study also explored the impact of defects on quantum efficiency, revealing a severe negative influence beyond a perovskite bulk defect density of 1×10^{17} cm^{-3}. Light intensity analysis demonstrated a correlation between incident light reduction and device performance decay. Capacitance–Voltage (C-V) and Mott–Schottky (M-S) have been analyzed during the study. Finally, the total recombination of the optimized device concerning thickness has been analyzed along with the dark J-V characteristics. The comprehensive insights gained from this work are anticipated to accelerate the fabrication of mixed Ge-Sn based PSCs with improved efficiency, paving the way for commercialization in the photovoltaic industry**.**

Keywords: Perovskite Solar Cells (PSCs), Germanium–Tin (Ge–Sn) Perovskite, Solar Cell Simulation, SCAPS-1D, Power Conversion Efficiency (PCE).

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