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Simulation and analysis of high-performance HTL-SrZrS₃ based perovskite solar cells: Comparative study

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To address the stability and toxicity issues of halide perovskites, we proposed chalcogenide perovskites as an alternative family of materials with the intention to replace halide perovskites for photovoltaic and other optoelectronic applications. Zr-based chalcogenides AZrS₃ (A=Ba, Ca, or Sr) are the most studied family of chalcogenide perovskites for optoelectronic properties, due to their low cost, high absorption coefficients, and high Power Conversion Efficiency (PCE) compared to that of organo-metal halide perovskite solar cells. A device simulation of SrZrS₃ as an absorbing material solar cells, as well as a proposal of low-cost Hole Transport Materials HTMs (Cu₂O, CuSCN, and NiOx), were performed by using SCAPS-1D software. Parameters such as (thickness, doping concentration, and temperature) for each configuration are varied in order to inspect their impact on the device performance. As a result, we have found that for SrZrS₃, the optimized configuration is: Au (metal back contact)/NiOx (HTM)/SrZrS₃ (Absorber)/ZnO (ETM)/FTO (Fluorine doped Tin Oxide), which delivered at 300 K: PCE of 14.64 %, V_{OC} (Open Circuit Voltage) of 1.20 V, J_{SC} (Short Circuit current density) of 22.10 mA/cm², and FF (Fill Factor) of 55.31 %.

Abstract Category

Materials Physics

Author: Ms CHAWKI, Najwa (Faculty of Sciences, Mohammed V University in Rabat,)

Presenter: Ms CHAWKI, Najwa (Faculty of Sciences, Mohammed V University in Rabat,)

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