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Lead-Free Inorganic Cesium Tin-Germanium Triiodide Perovskites for Photovoltaic Application

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Abstract : The toxicity of lead associated with the lifecycle of perovskite solar cells (PSCs(is a serious concern which may prove to be a major hurdle in the path toward their commercialization. The current proposed lead-free PSCs including Ag(I), Bi(III), Sb(III), Ti(IV), Ge(II), and Sn(II) low-toxicity cations are still plagued with the critical issues of poor stability and low efficiency. This is mainly because of their chemical stability. In the present research, utilization of all inorganic CsSnGeI₃ based materials offers the advantages to enhance resistance of device to degradation, reduce the cost of cells, and minimize the carrier recombination. The presence of inorganic halide perovskite improves the photovoltaic parameters of PCSs via improved surface coverage and stability. The inverted structure of simulated devices using a 1D simulator like solar cell capacitance simulator (SCAPS) version 3308 involves TCOHTL/Perovskite/ETL/Au contact layer. PEDOT:PSS, PCBM, and CsSnGeI₃ used as hole transporting layer (HTL), electron transporting layer (ETL), and perovskite absorber layer in the inverted structure for the first time. The holes are injected from highly stable and air tolerant Sn_{0.5}Ge_{0.5}I₃ perovskite composition to HTM and electrons from the perovskite to ETL. Simulation results revealed a great dependence of power conversion efficiency (PCE) on the thickness and defect density of perovskite layer. Here the effect of an increase in operating temperature from 300 K to 400 K on the performance of CsSnGeI₃ based perovskite devices is investigated. Comparison between simulated CsSnGeI₃ based PCSs and similar real testified devices with spiro-OMeTAD as HTL showed that the extraction of carriers at the interfaces of perovskite absorber depends on the energy level mismatches between perovskite and HTL/ETL. We believe that optimization results reported here represent a critical avenue for fabricating the stable, low-cost, efficient, and eco-friendly all-inorganic Cs-Sn-Ge based lead-free perovskite devices.

Keywords : hole transporting layer, lead-free, perovskite solar cell, SCAPS-1D, Sn-Ge based
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