Mathematical Modeling and Optimization of Highly Efficient Nontoxic All-Inorganic CsSnGeI3-Based Perovskite Solar Cells with Oxide and Kesterite Charge …	
Authors	**Muhammad Noman, Ihsan Nawaz Khan, Affaq Qamar, Khalid AlSnaie, Hassan M Hussein Farh**
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Abstract: Despite exceptional optoelectronic properties and rapidly increasing efficiency of perovskite solar cells (PSCs), the issues of toxicity and device instability have hampered the commercialization of this renewable energy technology. Lead (Pb) being the main culprit creates major environmental risks and therefore must be replaced with a nontoxic material such as tin (Sn), germanium (Ge), etc. Moreover, replacing organic cations in the perovskite's ABX3 structure with inorganic ones like cesium (Cs) helps aid the stability issues. This study uses six different kesterite-based hole transport layers (HTLs) and three different metal oxide-based electron transport layers (ETLs) to numerically simulate and optimize all-inorganic CsSnGeI3 PSCs. Metal oxide ETLs are used in this study due to their large band gap, while kesterite HTLs are used due to their excellent conductive properties. All of the simulations are performed under standard testing conditions. A total of 18 novel planar (n-i-p) PSCs are modeled by the combination of various charge transport layers (CTLs), and the device optimization was done to enhance the power conversion efficiencies (PCEs) of the PSCs. Furthermore, the effect of CTLs on the energy band alignment, electric field, quantum efficiency, light absorption, and recombination rate is analyzed. Additionally, a detailed analysis of the impact of defect density (Nt), interface defects (ETL/Perv, Perv/HTL), temperature, and work function on the functionality of 18 different CsSnGeI3-based PSCs is conducted. The simulation findings demonstrate that SnO2/CsSnGeI3/CNTS is the most efficient optimized PSC among all of the simulated structures, with a PCE of 27.33%, Jsc of 28.04 mA/cm2, FF of 85%, and Voc of 1.14 V.

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