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| **Title:** | Optimization of a high-performance lead-free cesium-based inorganic perovskite solar cell through numerical approach | | |
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| **Published Journal Name:** | Heliyon | | |
| **Type of Publication:** | Journal | | |
| **Volume:** | 8 | Issue | 11 |
| **Publisher:** | Elsevier | | |
| **Publication Date:** | Nov 16, 2022 | | |
| **ISSN:** | 2405-8440 | | |
| **DOI:** | https://doi.org/10.1016/j.heliyon.2022.e11719 | | |
| **URL:** | https://www.cell.com/heliyon/fulltext/S2405-8440(22)03007-9 | | |
| **Other Related Info.:** | Page e11719 | | |
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| **Abstract:** |  |
| In this work, an ultra-thin (0.815 μm) lead-free all-inorganic novel PV cell structure consisting of solid-state layers with the configuration SnO2/ZnOS/CsGeI3/CZTSe/Au has been optimized using SCAPS-1D simulator. ZnOS electron transport layer (ETL) has been deployed and various hole transport layer (HTL) material candidates have been considered to find the most suitable one in order to get the maximum possible power conversion efficiency (PCE). The simulation begins with the optimization of the thickness of the ZnOS buffer layer, followed by an analysis of HTL and ETL doping concentrations, thickness and bandgap optimization of absorber layer. The maximum permissible defect density at the ZnOS/CsGeI3 interface and the bulk defect density of the absorber layer (CsGeI3) are also investigated. It is also found that when the temperature rises, short circuit current density (Jsc) rises by 1.43 mA/K and open-circuit voltage (Voc) degrades by 2 mV/K. The optimized structure results in a PCE of 26.893% with Jsc, Voc, and fill factor (FF) of 28.172 mA cm−2, 1.0834 V, and 88.107% respectively. The cell performance parameters outperform those found in the recent literature. The simulated results of the proposed configuration are expected to be a helpful reference for the future implementation of a cost-effective and efficient all-inorganic perovskite PV cell. | |