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Comparative analysis using SCAPS 1-D software on the stability and toxicity of FAPbI3 and FASnI3 perovskites, aiming for environmental protection.

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Hybrid organic-inorganic perovskites such as $FAPbI_3$ (lead iodide and formamidinium) and $FASnI_3$ (tin iodide and formamidinium) are recognized as promising materials for the next generation of high-efficiency solar cells. $FAPbI_3$ is particularly valued for its stability and excellent optoelectronic properties. However, the toxicity of lead and the resulting environmental concerns drive the search for alternatives such as $FASnI_3$, where tin, a less toxic and more abundant element, replaces lead, which is the goal of this study. The lead-free structure simulated using SCAPS-1D software is as follows: FTO/TiO_2/$FASnI_3$/Spiro-OMeTAD/Ag. The research presented here shows that optimizing several parameters can achieve a power conversion efficiency (PCE) of 22.49%. In order to better compare this solar cell to $FAPbI_3$, various parameters affecting the device's performance, such as the thickness and doping of the ETL and HTL layers, as well as the total defect density of the absorbing layer, are studied and discussed. The best results obtained after optimizing the aforementioned parameters are: Jsc of 30.65 mA/cm², Voc of 0.8469 V, FF of 86.63%, and PCE of 22.49%. In this study, we used the SCAPS-1D simulator to model and evaluate the performance of photovoltaic devices based on these two perovskites. We chose TiO_2 as the electron transport layer (ETL) due to its wide band gap (˜3.2 eV), which effectively blocks holes and prevents their recombination with electrons, thus promoting better charge separation. Furthermore, the favorable alignment of the energy levels of TiO_2 with that of the perovskites facilitates the transfer of electrons to the silver (Ag) electrode [3]. For the hole transport layer (HTL), we chose Spiro-OMeTAD, whose valence band level is well aligned with that of the perovskites, thus facilitating hole extraction to the upper silver electrode. Using the SCAPS-1D simulator, we then compared the electrical and optical properties of the devices, focusing on key parameters such as short-circuit current density (Jsc), open-circuit voltage (Voc), fill factor (FF), and power conversion efficiency (PCE). Additionally, the structure studied in this paper could be a good candidate for future research on lead-free perovskite solar cells.

Primary author: TOURE, Sékou

Presenter: TOURE, Sékou

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