Modeling and Simulation of High Efficiency Eco-Friendly Perovskite-CZTSe_{1-x}S_x Solar Cell

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In the present paper, a Pb-free and eco-friendly perovskite solar cell (PSC) with a new structure of glass|TCO|TiO₂|CZTSe_{1-x}S_x|CH₃NH₃SnI₃|back contact has been modeled and simulated by SCAPS-1D package. To verify the simulation process, an experimental report on Pb-free PSC was simulated initially. Then, the costly Spiro-OMeTAD layer as the common hole-transport material (HTM) was eliminated. To overcome the possible deficiencies related to lacking of HTM plus management of the incident light, the economic and eco-friendly $Cu_2ZnSn(Se_{1-x}S_x)_4$ (CZTSe_{1-x}S_x) layer was added in the front of perovskite layer followed by optimizing the parameters. By optimization, the power-conversion efficiency of 17.57%, open-circuit voltage Voc of 0.85 V, short-circuit current density Jsc of 29.22 mA/cm², and fill factor of 70.47% were obtained. Meanwhile, very high quantum efficiency was achieved in the visible region of spectrum.

Keywords: solar cell, Pb-free perovskite, $CZTSe_{1-x}S_x$, non-toxicity, simulation.

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