ABSTRACT

Recently, lead-based perovskite solar cells have been mainly studied; however, these cells suffer from two main problems: the toxicity of lead and the instability of the devices, which limit their commercialization. Herein, a theoretical investigation of a lead-free perovskite solar cell based on formamidinium tin iodide ($HC(NH_2)_2SnI_3$) with the general architecture: glass/FTO/WS_2/$HC(NH_2)_2SnI_3$/HTL/Au is reported. All calculations are performed with the SCAPS-1D solar cell simulator. Two inorganic (CuSCN and Cu_2O) and two organic (P3HT and D-PBTTT-14) hole transport layer (HTL) materials are tested in this model. The effect of the external operating temperature and different metal work functions of the back contact of the cell on the overall performance of the devices is also studied. Simulations showed that, with the introduction of CuSCN, Cu_2O, and P3HT as HTLs, the device can attain a remarkable efficiency of ≈21%. All the modeled devices showed remarkable performance of above 20% at higher temperatures of 380–420 K but degraded slightly when this range is exceeded. Relatively cheaper Pt, Ni, and Pd metals perform better, thus, can replace gold. These simulation results can provide avenues and directions for future advancement of the performance of lead-free perovskite solar cells.