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Influence of Defects on the Photovoltaic Properties of Perovskite Semiconductor $CsSnI_3$ PENG XU, Fudan Unversity, SHIYOU CHEN, East China Normal University, HONGJUN XIANG, XIN-GAO GONG, Fudan University, SU-HUAI WEI, National Renewable Energy Laboratory — $CsSnI_3$ is a prototype inorganic halide perovskite that has recently been proposed as a photovoltaic material. Through first-principles calculations, we show that the concentration control of intrinsic defects is critical for optimizing the photovoltaic properties of $CsSnI_3$. Under a Sn-poor condition, high concentration of acceptor defects such as Sn or Cs vacancies can form easily and produce a high p-type conductivity, and deep level defects that can become electron-hole recombination centers, all have high energy. This condition is optimal for growing $CsSnI_3$ as hole-transport material in solar cells. In contrast, when Sn becomes richer, the concentration of acceptor defects decreases, so the p-type conductivity may drop to a moderate level, which can increase the shunt resistance and thus the efficiency of the solar cells with $CsSnI_3$ as the light absorber material (LAM). However, under the Sn-rich condition, the concentration of a deep-level donor defect Sn_I will increase, causing electron traping and non-radiative electron-hole recombination. Therefore, we propose that a moderately Sn-rich condition is optimal when $CsSnI_3$ is used as LAM.

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