Strain effects on electronic, optical properties and carriers mobility of Cs_2SnI_6 double perovskite: A promising photovoltaic material

B. Rezini[1], T. Seddik[1], R. Mouacher[1], Tuan Vu[2], Mohammed Batouche[3], and O.Y. Khyzhun[4]

[1]University of Mascara
[2]Ton Duc Thang University
[3]Université de Mascara
[4]National Academy of Sciences of Ukraine

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Abstract

Owing to the fascinating optoelectronic and photovoltaic properties, perovskite halide materials have attracted much attention for solar cells applications. Using the first-principles approaches, we present here results of calculations of the strain effects on electronic and optical properties as well as carriers mobility of Cs_2SnI_6 double perovskite. The calculated band gap energy of unstrained Cs_2SnI_6 is about 1.257 eV when using Tran-Blaha modified Becke Johnson (mBJ) exchange potential that is in fair agreement with experimental measurements. Under the applied strains, this band gap value increases up to 1.316 eV for -4% compressive strain and decreases till 1.211 eV for 4% tensile strain. This effect is mainly due to the fact that the conduction band minimum shifts under compressive and tensile strains. From carrier mobility calculations, we notice that under tensile strain both hole and electron carrier mobilitiy diminishes, whereas the carrier mobility increases by 25.7 % for electron and by 15 % for holes under -4% compressive strain. Moreover, the optical analysis reveals that applied strain can affect the optical properties of Cs_2SnI_6 perovskite.

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