Theoretical performance study of $Cs_2AgBi(I_{(1-x)}Br_x)_6$: a promising lead-free perovskite for photovoltaic technology

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Abstract

In recent years, there has been a great interest in the development of lead-free, stable and high efficiency perovskite materials. In our work, we studied a lead-free, inorganic and non-toxic double perovskite solar cell (PSC) based on $Cs_2AgBi(I_{(1-x)}Br_x)_6$ using ab-initio calculations density function theory (DFT) study. The stability, electronic and optical properties are studied and the transport properties have been calculated. Thus, we have evaluated the band gap of the $Cs_2AgBi(I_{(1-x)}Br_x)_6$ absorber by two approximations GGA-PBE and TB-mbj. We found that the values of absorptivity and dielectric constant also increase with increasing Br doping. These mixed halide compounds show stronger absorption coefficients from 300 to 600 nm, the lowest light absorption capacity is observed between 600 and 800 nm.

The performance of the compounds is simulated via SLME. To improve the performance of the device, we analyzed and optimized different parameters of the PSC: optimal thickness, defect density and band gap of the absorber by the numerical simulation method of perovskite solar cell using SCAPS-1D (solar cell capacitance simulator) software. Thus, the optimized values of the doping density for the absorber layer, HTL and ETL were determined; the device achieved a good PCE. Bi-based double mixed halide perovskite materials have provided great scope for a broad range of applications cells with the same high performance as lead-based perovskite. They can be obtained experimentally in future.

Keywords: *$Cs_2AgBi(I_{(1-x)}Br_x)_6$ absorber, DFT study, perovskite solar cells, Photovoltaic technology*

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