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Investigation of the potential of the double perovskite materials Cs_2BX_6 and $Cs_2BB'X_6$ as absorbers in single and tandem solar cells for high-efficiency photovoltaic conversion

Hayat Arbouz[1]✉

[1] *University Saad Dalhab Blida1,Department of Physics, Blida-Algeria*

Abstract

Recent years have seen an impressive development of lead-based perovskite absorber solar cells of the ABX_3 class, which have demonstrated high efficiencies competitive with other technologies. However, the toxicity and instability of these materials considerably reduce their advancement despite their high performance. To overcome these drawbacks, research into the development of stable, efficient perovskite cell technology has been stepped up, and lead-free, inorganic perovskite-based devices have emerged. The present study aims to explore the potential of non-toxic inorganic double perovskite materials of compositions Cs_2BX_6 and $Cs_2BB'X_6$, as absorber layers in single solar cells, or as top or bottom sub-cells, depending on the bandgap energy value, in double-junction tandem solar cells. The performance of single-junction cells based on the Cs_2BX_6 class of perovskites, such as Cs_2TiBr_6, Cs_2TeI_6 and Cs_2PtI_6, has been simulated using a proprietary model. The same applies to the class of $Cs_2BB'X_6$ perovskites such as Cs_2AgBiI_6, Cs_2AuBiI_6 and $Cs_2BiAuCl_6$.The results have been reported and discussed. As these materials have different bandgap energies, their respective solar cells can serve as lower or upper sub-cells in tandem configurations, depending on the value of each. Several combinations of tandem structures were proposed in this study, where the two-terminal configuration was used, showing improved efficiencies in excess of 25%.
This work is contributing to the development of high-efficiency solar cells based on stable and environmentally-friendly inorganic double perovskite absorbers.

Keywords: *Double-Perovskite, Solar Cell, Tandem Cell, Simulation*

✉ *arbouzhayet@yahoo.fr*