

Optoelectronic properties and symmetry analysis of halide lead-free double perovskites

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Hybrid organic-inorganic halide perovskites { ABX_3 with $A = CH_3NH_3$ (MA), NH_2CHNH_2 (FA), Cs, Rb ; $B = Pb$ and $X = Cl, Br$ or I } have become a very important class of materials for low-cost photovoltaic applications in the past few years. In 2016, the efficiency of a single-junction perovskite solar cell has reached 22.1%¹, getting close to the average efficiency of Al-BSF silicon cells in a short amount of time. Nevertheless, many issues are still worthwhile working on to obtain a non-toxic stable photovoltaic device. For instance, the presence of lead has led the community to search for alternative materials, which are both stable, earth abundant and environment-friendly. Replacing Pb with elements from the same periodic group (Sn, Ge...) has been widely investigated, but the instability of Sn^{2+} and Ge^{2+} based compounds is a serious obstacle for the development of lead-free architectures². More recently, double halide perovskites { $A_2B^I B^{III} X_6$ with $A = Cs, MA$; $B^I = K, Ag, In, Tl$ etc ; $B^{III} = Bi, Al, Ga, In$ etc and $X = Cl, Br$ etc} have opened a new path for the study of lead free perovskites systems³⁻⁴. Contrary to their halide lead perovskites analogues, the understanding of their optoelectronic properties is still in its infancy. We study in the present work several members of the double perovskites family (Cs_2AgInX_6 and Cs_2AgBiX_6 , with $X = Cl, Br, I$). Deep dielectric characterization is among others performed here using DFT calculations (using VASP, Crystal and Siesta codes) ; this type of study as proven to be necessary for the understanding of several type of halide perovskites regarding PV and photonic applications⁵.

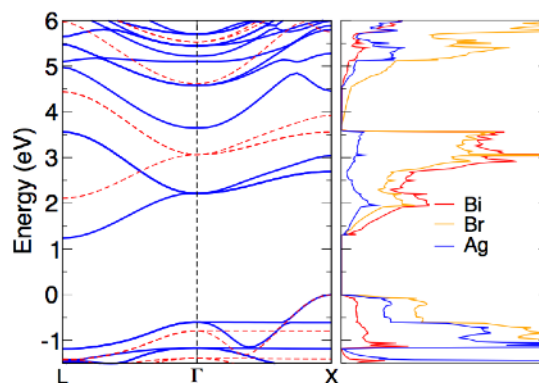


Figure. (left) Band diagram of $Cs_2AgBiBr_6$, calculated by DFT with HSE (red) and PBE (blue) functionals and without spin-orbit coupling. (right) corresponding PDOS calculated with PBE.

References

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