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PAPER

Deep insight into structural and optoelectronic properties of mixed anion perovskites

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Abstract

Here we present the optoelectronic properties of pure inorganic lead-free halide perovskites in the form of Cs_2AgBiX_6 (X = Br, Cl, F, I) using the density functional theory calculations on cubic phase (Fm $\bar{3}$ m) and tetragonal phase (I4/m). First, all the structures of the two phases were optimized at the PBE level. Structural, electronic, optical properties, phonon, and thermal properties of Cs_2AgBiX_6 in cubic (Fm $\bar{3}$ m) and tetragonal phases (I4/m) were obtained using the VASP code. Tetragonal phases of all compounds of the form Cs_2AgBiX_6, except $Cs_2AgBiBr_6$, are reported here for the very first time. Among all the Cs_2AgBiX_6 (X = F, Cl, Br, I) structures, the cubic phase of $Cs_2AgBiBr_6$ was seen to have the highest absorption coefficient along with prominent electronic features that are favorable for optoelectronic applications. Thus, the cubic phase of $Cs_2AgBiBr_6$ was selected as the host lattice and bromine atoms were partly replaced with chlorine and iodine atoms. Electronic and optical properties of these mixed halide compounds of $Cs_2AgBiBr_{6-x}F_x$, $Cs_2AgBiBr_{6-x}Cl_x$, and $Cs_2AgBiBr_{6-x}I_x$ where x = 1, 2, 3, 4, 5 are investigated with hybrid functional HSE06 level. The electronic structure revealed that these mixed compounds exhibited indirect band gap nature regardless of the halide substitution (different x concentration) and the band gap of $Cs_2AgBiBr_6$ could be varied with the substitutions of fluorine, chlorine, and iodine atoms. Our in-depth analysis shows that $Cs_2AgBiBr_6$ and their mixed halides have the potential to become active double perovskite materials for photovoltaic applications and as photocatalysts for water splitting.