Supporting Information

Potential Applications of Halide Double Perovskite Cs_2AgInX_6 (X = Cl, Br) in Flexible Optoelectronics: Unusual Effects of Uniaxial Strains

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Table S1. Lattice constants (a=b=c) (in unit of Å) obtained by different methods, and bond lengths (in unit of Å), elastic constants (in unit of N/m) and band gaps (in unit of eV) calculated by LDA method for Cs_2AgInX_6 (X= Cl, Br). For comparison, the values calculated from previous studies and experiments are also listed.

	Lattice constant						Bond length		Elastic constant	Band gap
	LDA	Experiment	HSE	PBE	PW91	PBE0	In-X	Ag-X		
$Cs_2AgInCl_6$	10.22, 10.2[1]	10.47	10.62[1]	10.65[1]	10.65	10.68	2.51	2.59	71.02	0.65, 2.1-3.3[1]
$Cs_2AgInBr_6$	11.43, 11.16[2], 11.20[3]		11.20[4]	11.60	11.60	11.58	2.81	2.90	67.73	0.58 1.5[2], 1.33[3]

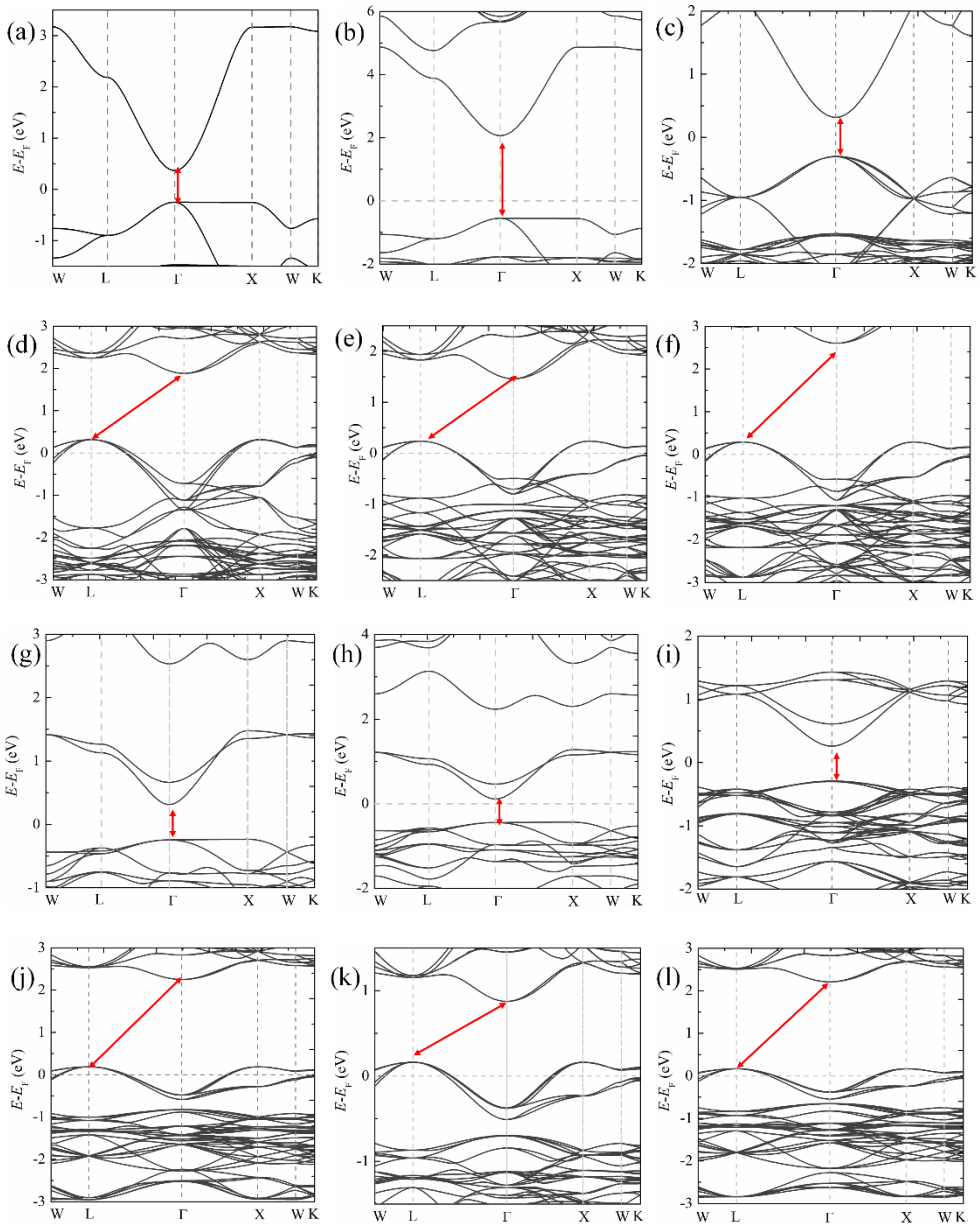

Figure S1. Band structures of $Cs_2AgInCl_6$ primitive cell obtained by (a) LDA and (b) HSE functionals, respectively. Band structures of $Cs_2AgInCl_6$ unit-cell obtained by (c) LDA, (d) GGA-PBE, (e) PBE0, (f) GGA-PW91 methods, respectively. Band structures of $Cs_2AgInBr_6$ primitive cell obtained by (g) LDA and (h) HSE functionals, respectively. Band structures of $Cs_2AgInBr_6$ unit-cell obtained by (i) LDA, (j) GGA-PBE, (k) PBE0, (l) GGA-PW91 methods, respectively.

It can be found that the band structures of Cs_2AgInX_6 (X=Cl, Br) calculated by

GGA-PBE, GGA-91, PBE0 methods show indirect band gap characters, which is inconsistent with previous reports [1,4,5]. That is because band edges of Cs_2AgInX_6 (X=Cl, Br) are sensitive to the lattice constants (such phenomenon is analyzed in detail in the following section) which are difficult to be accurately obtained by these methods, as listed in Table S1. While the band structures of Cs_2AgInX_6 (X=Cl, Br) perovskite obtained by LDA and HSE corrected methods [1,4,5] are similar, except for the band gaps, suggesting that LDA method is sufficient to understand the electronic properties of Cs_2AgInX_6 (X=Cl, Br) perovskite. Thus, the physical properties, except for the band gap, of Cs_2AgInX_6 (X=Cl, Br) in the following section are calculated by LDA method.

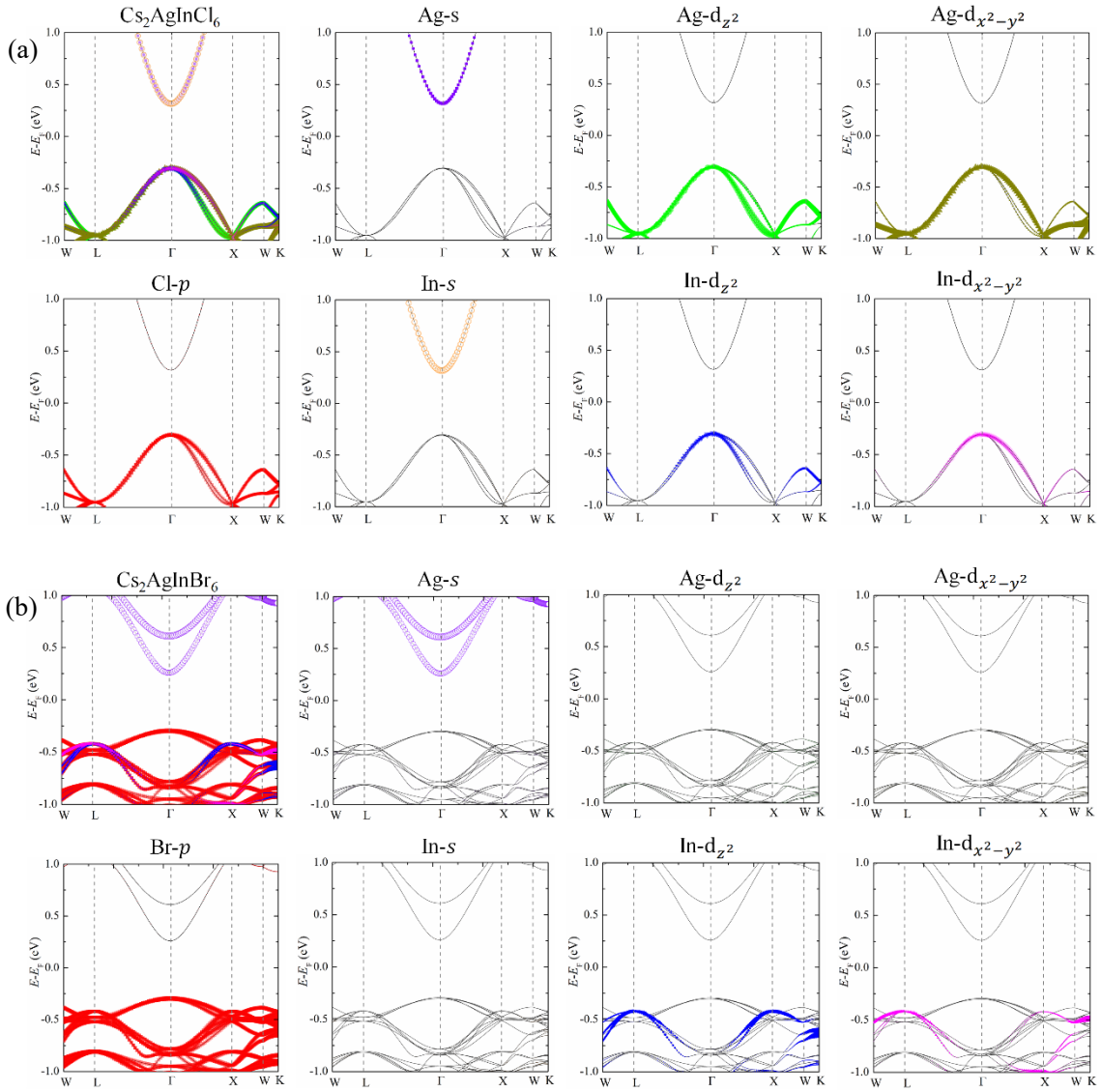

Figure S2. Orbital-projected band structures for (a) pure $Cs_2AgInCl_6$ and (b) pure $Cs_2AgInBr_6$. The vertical color belt represents the strength of corresponding orbital contributions.

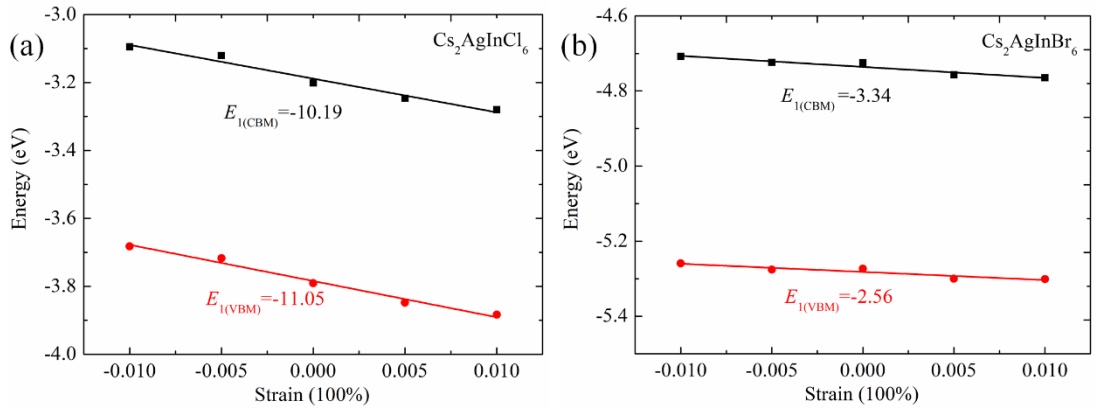

Figure S3. Energy shifts of CBM and VBM of (a) $Cs_2AgInCl_6$ and (b) $Cs_2AgInBr_6$ under strains, respectively. The slopes of these lines are the corresponding deformation potentials.

References

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