Electronic, Magnetic and Optic Properties in Halide Perovskites CsPbX3 (X= F, Cl, I)

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Abstract : We performed first-principle calculations, the full-potential linearized augmented plane wave (FP-LAPW) method is used to calculate structural, optoelectronic and magnetic properties of cubic halide perovskites CsPbX3 (X= F,I). We employed for this study the GGA approach and for exchange is modeled using the modified Becke-Johnson (mBJ) potential to predicting the accurate band gap of these materials. The optical properties (namely: the real and imaginary parts of dielectric functions, optical conductivities and absorption coefficient absorption make this halide perovskites promising materials for solar cells applications.

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