

## MS14-P02 | FIRST-PRINCIPLES INVESTIGATION OF STRUCTURAL, ELECTRONIC AND OPTICAL PROPERTIES OF $\text{CsPb}(\text{I}_{1-x}\text{Br}_x)_3$ ( $x = 0.0 - 1.0$ ) COMPOUNDS

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The structural, electronic and optical properties of the  $\text{CsPb}(\text{I}_{1-x}\text{Br}_x)_3$  ( $x = 0, 0.25, 0.33, 0.5, 0.66, 0.75$  and  $1$ ) were investigated using the full potential augmented plane wave (FP-LAPW) scheme in the frame of generalized gradient approximation (GGA). The two exchange potentials, PBE-GGA and mBJ-GGA are used to study the electronic and optical properties. In this study, we have observed an increase in band gap values by  $0.56$  eV with increasing the concentration of Br atoms in  $\text{CsPb}(\text{I}_{1-x}\text{Br}_x)_3$  alloys whereas the refractive indices, reflection and real part of dielectric function have reverse effect. It is noted that all of the compounds are wide and direct band gap semiconductors with band gap located at A-symmetry point. The optical properties of these compounds like optical conductivities, absorption coefficients, real and imaginary parts of dielectric functions, refractive indices, extinction coefficients, and reflectivity, are also calculated. The direct band gap nature and high absorption power of these compounds in the visible ultraviolet energy range imply that these perovskites can be used in optical and optoelectronic devices working in this range of the spectrum by replacing I by Br.