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First Principle Calculations of the Structural and Optoelectronic Properties of Cubic Perovskite CsSrF3

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Abstract : We have investigated the structural, electronic and optical properties of a compound perovskite CsSrF3 using the full-potential linearized augmented plane wave (FP-LAPW) method within density functional theory (DFT). In this approach, both the local density approximation (LDA) and the generalized gradient approximation (GGA) were used for exchange-correlation potential calculation. The ground state properties such as lattice parameter, bulk modulus and its pressure derivative were calculated and the results are compared whit experimental and theoretical data. Electronic and bonding properties are discussed from the calculations of band structure, density of states and electron charge density, where the fundamental energy gap is direct under ambient conditions. The contribution of the different bands was analyzed from the total and partial density of states curves. The optical properties (namely: the real and the imaginary parts of the dielectric function ε(ω), the refractive index n(ω) and the extinction coefficient k(ω)) were calculated for radiation up to 35.0 eV. This is the first quantitative theoretical prediction of the optical properties for the investigated compound and still awaits experimental confirmations.

Keywords : DFT, fluoroperovskite, electronic structure, optical properties
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