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RESEARCH ARTICLE

Density functional theory based study of the physical properties of cesium based cubic halide perovskites $CsHgX_3$ (X=F and Cl)

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Summary

Structural, elastic, electronic, and optical properties of Cs-based halide perovskite compounds $CsHgX_3$ (X=F and Cl) are computed in the framework of density functional theory (DFT). The obtained optimized lattice parameters are found to agree with available experimental and other theoretical data. Elastic parameters, such as anisotropic factor, bulk modulus, elastic constants, Pugh's ratio, and Poisson's ratio, are predicted. It is observed from the elastic properties measurements that these compounds are ductile, anisotropic, and mechanically stable. Band structures and density of states (DOS) are performed for the computation of electronic properties and it is found that the calculated bandgap of $CsHgF_3$ is of an indirect and semiconductive nature, while $CsHgCl_3$ reveals metallic nature. For more clarification of electronic properties, the DOS presents the different contributions of valence states to valence and conduction bands. Optical properties, such as real and imaginary parts of dielectric functions, reflectivity, extinction coefficients, absorption coefficients, optical conductivity, and refractive indices, are also calculated in the energy range 0 to 30 eV. From the optical properties, it is found that these materials possess high absorption and refractive index, due to which it can be deemed as a suitable candidate for optical lenses and optical coating materials.