The elastic, electronic and optical properties of RbCaX3 (X = F, Cl) compounds

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Abstract

The structural, elastic, chemical bonding, electronic and optical properties of the cubic perovskites RbCaX3 (X = F, Cl) compounds are obtained by the full-potential linear augmented plane wave (FP-LAPW) method based on the density functional theory. The calculated lattice constants and bulk moduli within GGA agree with previous calculations. It is found that the bulk modulus decreases as the lattice constant increases when traversing from F to Cl in RbCaX3. Both compounds are found to be elastically stable and anisotropy from the analysis of elastic constants. The analysis of Poisson's ratio, Cauchy pressure and Pugh's index ratio indicate that the RbCaF3 is brittle compound while the RbCaCl3 is ductile compound. The Debye temperature for the RbCaX3 compound evaluates from the average sound velocity. Both compounds are found to have the indirect band-gap (M-Gamma) from calculating the band structure. The bonding nature of RbCaX3 compounds is ionic with a minute covalent bonding. The optical properties are calculated for radiation up to 30 eV. The main peaks of the optical spectra are discussed in terms of the calculated electronic structure. A beneficial optoelectronic and optics technology is predicted from optical spectra.

Keywords

Author Keywords: Brittleness and ductility; elastic properties; anisotropy; electronic structure

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