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First Principles Calculations of the Structural and Electronic Properties of Matlockite CaFI Compound

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The full potential linearized augmented plane wave (FP-LAPW) method within density functional theory [1] is applied to study, for the first time, the structural and electronic properties of CaFI and to compare them with CaFCl and CaFBr, all compounds belonging to the tetragonal PbFCl structure group with space group P4/nmm. We used the generalized gradient approximation (GGA) [2] based on exchange–correlation energy optimization to calculate the total energy and also the Engel–Vosko GGA formalism, which optimizes the corresponding potential for band structure calculations. Ground state properties such as the lattice parameters, c/a ratio, bulk modulus, pressure derivative of the bulk modulus and cohesive energy are calculated as well as the optimized internal parameters, by relaxing the atomic position in the force directions. The variations of the calculated interatomic distances and angles between different atomic bonds are discussed. CaFCl was found to have a direct band gap at 5 whereas CaFBr and BaFI have indirect band gaps. From these computed bands, all three materials are found to be insulators having band gaps of 6.28, 5.46 and 4.50 eV, respectively. We also calculated the valence charge density and the total density of states at equilibrium volume for each compound. The results are in reasonable agreement with the available experimental data.