ABSTRACT

The influence of metal doping (Mg and Be) on phase transition, electronic band structure, and their effects on the optical, elastic, and mechanical characteristics of RbCaF3 have all been examined in depth theoretically. We conducted this analysis to discover more about these qualities. These features were investigated using the PBE functional and the Generalized Gradient Approximation (GGA). It is studied how the most current estimated measurements compare to older theoretical work. Even when doped with 1.40% Mg and Be atoms, the structure of RbCaF3 remains cubic; however, when the doping concentration is raised to 4.22% or 7.04%, a pseudo-cubic tetragonal phase is observed. Every time doping occurs, the band gap decreases consistently and substantially. The nature of this phenomenon is revealed to be indirect in the cases of Mg (1.40 and 4.22%) and to be directly related to the symmetry points. To comprehend the narrowing of the band gap, consider the total density of states (TDOS), partial density of states (PDOS), and elemental partial density of states (EPDOS). Electronic states are used to talk about the optical properties. Following investigation of Mg with 1.40% and 4.22%, the indirect energy band gap is found. Examined is the determination of the actual and fictitious components of the dielectric functions. With Mg-doping and Be-doping, the optical response of the doped material exhibits a red shift in the absorption edge while the refractive index decreases from 1.809 to 1.668. A compound's electrical structure, optical properties, and mechanical characteristics would alter as a result of doping with magnesium, beryllium, or either element. These modifications would make the doped compound a strong candidate for improved optimization as a UV filter because it absorbs in the UV region.