

Doping  $\text{TlCaF}_3$  with different elements (Cl, Br, and I) at varying concentrations is shown to drastically modify the phase transition, electrical band structure, optical, elastic, and mechanical properties of the material. This is proved by the results of the research. Several different experiments provide evidence to support this conclusion. When it is in its pure form,  $\text{TlCaF}_3$  maintains its cubic structure. It undergoes a transformation from a cubic phase to a pseudocubic tetragonal phase with doping concentrations ranging from 2.81 percent to 5.63 percent of all doping components. When impurity atoms are added, a systematic and significant narrowing of the bandgap is observed. The manner in which this occurs depends on the symmetrical positions of the atoms, and it can be either direct or indirect. The total, partial and elemental density of states (DOS), which is affected by structural differences, can help alleviate some of the concerns regarding the narrowing of the bandgap. The optical response of a material that has been doped displays a decrease in the absorption edge, which implies a decrease in the electronic band gap. This is because doping causes a decrease in the electronic band gap. This happens despite the fact that doping of any kind causes an increase in the refractive index. The determined elastic constants for the cubic and tetragonal structures are comparable to one another, which is consistent with the mechanical stability criteria for each doping quantity. In addition, by making use of elastic parameters, it is possible to estimate the one-of-a-kind mechanical characteristics of undoped and doped compounds in order to evaluate their ductility and brittleness. In addition, the presence of their absorption spectra in the ultra violet region and the modification in structural, electrical, optical, elastic, and mechanical properties would make them an excellent candidate for enhanced optimization in ultra violet filters (UVF). This would be the case due to the fact that Cl, Br, and I-doping would render them appropriate for this purpose.