Abstract

Cubic Scandium Triflouride (ScF3) is a material that contracts when exposed to heat. Not many materials are known to behave this way. Such a material has many interesting technological applications yet some of its properties are yet to be fully explored using ab initio methods. This paper engaged the state-of-the-art ab initio methods to study the Structural and Mechanical properties of ScF3 at ambient conditions. All calculations were done within the Density Functional Theory (DFT) framework and a plane wave basis set as implemented in the QUANTUM ESPRESSO computer code. A comparison with previous DFT and Experimental studies was done. The Projector Augmented Wave pseudo-potentials were used to describe the core-valence electron interactions with the GGA (PBE,PBEsol,PW91,WC) and LDA chosen for the exchange –correlations. The cubic ScF3 was modeled using 4-atoms. The calculated lattice parameters for cubic ScF3 were found to be in good agreement with previous studies and differed by -1.17% to 1.07% from the experimental value. The calculated elastic constants (C11=231.65GPa to 280.15GPa, C12=16.41GPa to 18.18GPa and C44=17.74GPa to 18.61GPa) were also in agreement with the existing cited data. This paper points out the fact that ScF3 is a ductile material at ambient conditions and will deform under tensile stress.

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