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An investigation on lattice vibration and negative thermal expansion of ScF3 and other D09 structure materials

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A large negative thermal expansion (NTE) was discovered in simple cubic scandium trifluoride (ScF3) over a wide range of temperatures. The underlying mechanism has been explained by Li et al. [1] in terms of the vibration mode with the transverse motion of F atoms to their bond direction which behaves as quantum quartic oscillator. In this work, frozen phonon calculations with first-principles methods based on the density functional theory (DFT) have been performed to validate the individual modes in the phonon density of states and also investigate the anharmonic contribution on the potential energy of those vibrations in ScF3. The results showed the quartic potential for the traverse mode of F atoms. In addition, the anharmonic contribution on potential energy of some materials with D09 structure (ReO3, UO3, MoF3, TaF3 and NbF3) has been studied in comparison with ScF3. It has been found that the degrees of anharmonicity significantly depend on the bonding character between the two atomic species which can be described by simple spring-mass model.

[1] C. W. Li, X. Tang, J. A. Muñoz, J. B. Keith, S. J. Tracy, D. L. Abernathy, and B. Fultz, Phys. Rev. Lett. 107, 195504 (2011).

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