Pressure-dependent structural, elastic, electronic and vibrational studies of Sr_2InSbO_6 from first principles simulations.

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Abstract

Perovskite materials have interesting and unusual physical properties that have been studied a lot for both real-world applications and theoretical modelling. The science of perovskites and how they can be used, has been a large area of research that has led to many new device ideas based on revolutionary discoveries. Double perovskite compounds, first identified in the 1950s, are remarkable for their characteristics and the wide range of uses they find in industry. A2BB0O6 double perovskite oxides have gained considerable attention over the past two decades due to their extensive structural diversity, as well as potential technological applications in microwave dielectric ceramics, optoelectronic device materials The ideal double perovskite structure of the general formula A2BB0O6 is derived from the perovskite structure ABO3 when the octahedrally coordinated two B-cations are occupied by a B cation and a B0-cation in an ordered 1:1 way, where B and B0 cations are largely different in charge or size.

First-principles calculations have been performed to study the structural, elastic, electronic, and lattice dynamical properties of Sr_2InSbO_6. Our first-principles density functional theory, DFT, calculations were performed with the pseudo-potential plane-wave method as implemented in the Vienna ab initio Simulations Package, VASP.In this work, we present a study of the evolution of the structural, vibrational, elastic, and electronic properties under hydrostatic pressure.