The Relativistic Study of Structural, Electronic, and Phononic Properties of GaBi Compound at Under-Pressure Phases

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Abstract

In the present work, the ab-initio calculations based on the pseudo-potential plane wave method were performed to fully relativistically study the structural, electronic, and phononic properties of GaBi compound in the CsCl and NaCl (RS) phases. This compound has the stable zinc blende phase that in this phase is semi-metal while in the under-pressure, in other words, in CsCl and NaCl phases, it has a metallic behavior. It is determined from the entropy graph in terms of the pressure that the spin-orbit interaction affects the order of the transition phase of this composition. By analyzing the phonon dispersion curves, it can be found that GaBi compound in these phases is unstable.

Keywords: gallium-bismuth, ab-initio calculations, spin-orbit coupling, under-pressure phases

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