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The effect of pressure and spin orbit interaction on topological phase and phonon dispersion of LuX (X= Sb, Bi) compounds

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Abstract

In this paper, the topological phase of LuX (X= Sb, Bi) compounds under hydrostatic and biaxial pressures is investigated based on first principles of density functional theory by WIEN2k package. To find out the Z_2 topological invariants of centrosymmetric compounds with the time reversal symmetry, the Bloch functions parity analysis can be used via electronic band structure calculations. So in this paper the Z_2 topological invariants of the LuX (X= Sb, Bi) compounds with the time reversal and inversion symmetries are calculated using this approach. The results show that the *d-p* band inversion can be occurred in these compounds due to spin orbit interaction and appropriate pressure. These compounds have the strong electronic interaction due to their large *d*-electronic orbitals near the Fermi energy. The dynamic stability of these compounds is verified by phonon modes analysis. The surface states topological phase of these compounds are investigated based on the band structure calculations.

Keywords: Density functional theory, LuX (X= Sb, Bi), Topological phase, Spin orbit interaction, Pressure, Phonon modes