Topological Phase Transition Associated With Structural Phase Transition in Ternary Half Heusler Compound LiAuBi

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Discovering new materials is a key aspect of semiconductor physics for sustaining the continuous progress and improvements in current electronic devices. The discovery of the non-trivial topological phase was a deviation from the conventional classification of materials, i.e., metals, insulators, and semiconductors. The discovery of the topological phase has become a center of attention in the condensed matter community due to riveting underlying physics and opening vast opportunities for their applications in next-generation spintronic devices. The topological phase in the materials is realized by time-reversal protected surface states, a distinctive quantum state of matter for the transport of spins. In recent years, immense research ploughed into discovering many such new materials at the horizon of physics and material science [1]-[3]. More recently, the search has been extended to ternary compounds, particularly non-centrosymmetric half Heusler compounds. Over the decade, HH compounds have made considerable development in thermoelectric conversion technology. Half Heusler compounds with 18 valence electrons, such as RNiSn (R = Hf, Zr, Ti), were found to have significant values of the Seebeck coefficient and power factor, which are essential in determining the thermoelectric (TE) efficiency of a material [4]-[5]. The reason behind this was the small band gap of the compounds with high charge carrier density. Externally doping or applying strain resulted in enhancement of the efficiency of a TE material. In this work, we report detailed theoretical investigations of topological phases in non-centrosymmetric half Heusler compound LiAuBi upto a pressure of 30 GPa [6]. It is found that the compound forms into a dynamically stable face centered cubic (FCC) lattice structure of space group F¯43m (216) at ambient pressure. The compound is topologically non-trivial at ambient pressure, but undergoes a quantum phase transition to trivial topological phase at 23.4 GPa. However, the detailed investigations show a structural phase transition from FCC lattice (space group 216) to a honeycomb lattice (space group 194) at 13 GPa, which is also associated with a non-trivial to trivial topological phase transition. Further investigations show that the compound also carries appreciable thermoelectric properties at ambient pressure. The figure of merit (ZT) increases from 0.21 at room temperature to a maximum value of 0.22 at 500K. The theoretical findings show its potential for practical applications in spintronics as well as thermoelectricity, therefore LiAuBi needs to be synthesized and investigated experimentally for its applications.

References

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