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Pressure induced structural and topological phase transition in ternary compound LiAuBi

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The study of topological semimetals and insulators have become a keen interest in the field of solid-state physics which are known to possess properties that enhances the performance of a thermoelectric (TE) material1,2 In our study, we have performed detailed theoretical investigations of topological phases in non-centrosymmetric half Heusler compound LiAuBi upto a pressure of 30 GPa. It is found that the compound forms into a dynamically stable face centered cubic (FCC) lattice structure of space group 216 at ambient pressure. The presence of spin-orbit coupling results in the s-p band-inversion near the Fermi level and thus may be categorized as topological semi-metals. 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.\ To understand its TE performance, transport properties are studied using Boltzmann transport theory, which show that the compound also carries appreciable thermoelectric properties at ambient pressure. The theoretical findings pave its path for practical applications in spintronics as well as thermoelectricity, therefore LiAuBi needs to be investigated experimentally.

Biography

Anita Yadav is a Ph.D. scholar at Departmnet of Physics, Indian Institute of Technology (IIT) Ropar, India. She works on first principles investigation of 2D and 3D ternary compounds for their electronic band structures, magnetic, and thermoelectric properties.

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