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Topological behaviour of Ternary non-symmorphic crystals KZnX (X=P,As,Sb)

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The discovery of topological insulators (TIs) and topological semimetals has attracted tremendous interest in condensed matter physics and material science. New topological phases of materials have provided new routes to developing technological applications in nanoelectronics, spintronics and topological quantum computing platforms [1]. The search for TIs has been received a great advantage from the topological band theory. It has been shown that, on materials front all TIs are narrow gap semiconductors and in the presence of strong spin-orbit coupling, their electronic structure is characterized by a band-inversion. In TIs such band inversion occurs at an odd number of time reversal invariant momenta (TRIMs) due to the switching of bands with opposite parity around the Fermi level [2]. Very recently, it has been theoretically proposed that several materials are a new type of topological insulators (TIs) protected by non symmorphic symmetry and this is further confirmed experimentally as well [1]. In this work we propose an unexplored class of ternary Zintl phases KZnX (X= P, As, Sb) investigated using Density Functional theory (DFT). The ab initio studies reveal that all the three materials are direct band gap semiconductors at ambient conditions. In this work we theoretically demonstrate that KZnX can be driven into different topological phases under pressure. Whereas by applying strain the compounds can be realized as topological insulators. This is confirmed by the observed non trivial topological character in the electronic band structure of the present ternary systems. For accurate determination of the low energy band topology, modified Becke-Johnson (mBJ) [3] exchange potential was used by incorporating spin-orbit coupling. The concomitant change of electronic band shapes as a function of pressure indicates a semi-metallic nature in KZnX (X=P, As, Sb) at 30GPa, 21GPa and 11GPa respectively. Based on an analysis of parity eigenvalues, we anticipate that a band inversion occurs between Zn-s and X-p states thus demonstrating a weak topological behaviour in semi metallic states. A weak non trivial topologically insulating phase is realized in strained KZnAs (18%) and KZnSb (10%) which appears due to overlapping of Zn-s and X-p orbitals. Since the proposed class of materials is extremely rich, much wider flexibility is provided in designing them by tuning the band gap. Our work highlights that pressure and strain can trigger topological phases in non-symmorphic trivial band insulators and that the spin orbit interaction plays a significant role in this consequence. This study paves a way to realize semi-metallic and topological insulating states in non-symmorphic ternary semiconductors, which have not been experimentally demonstrated so far.

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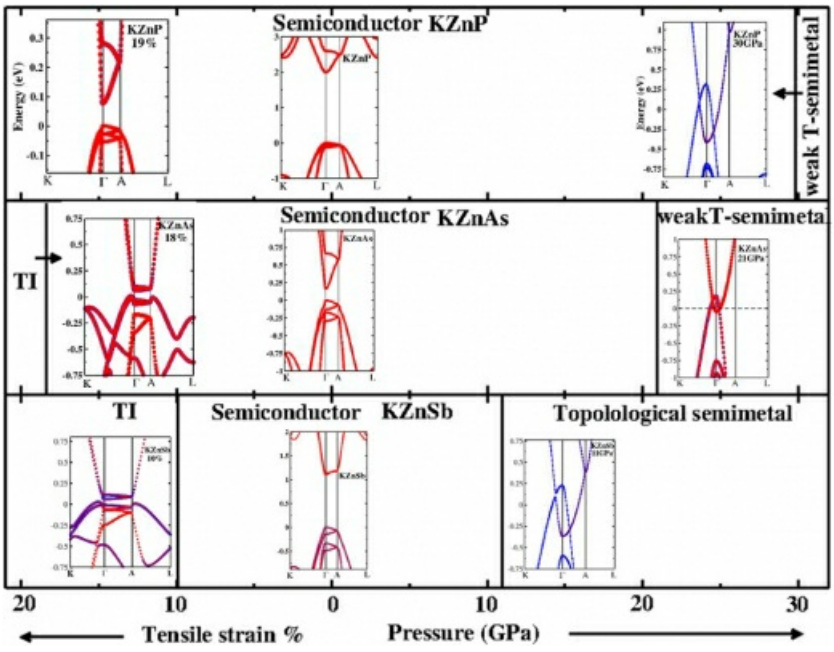

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