Non-trivial topological phases in transition metal rich half-Heusler Oxides

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Topological Insulators with gapless surface states and insulating bulk in non-centrosymmetric cubic systems have been extensively explored following the discovery of two-dimensional quantum spin hall effect in zincblende HgTe.[1,2] In such systems the negative band inversion strength function E_{BIS} (= $E_{\Gamma 6}$ - $E_{\Gamma 8}$ < 0) governs the robustness of the non-trivial topological states at ambient conditions.[3] Hence, realizing large negative values of E_{BIS} has been a guiding motivation of several investigations reported in literature. Here, we present a material design approach which can be employed to realize large negative values of E_{BIS} in cubic materials such as Half-Heusler (HH) oxides with 18 valence electron configurations.[4] We explore, α-, β-, and γ-phase (by placing transition metal atom at different Wyckoff positions) in HH oxides XYO (X = Li, K, Rb; Y = Cu, Ag, Au) for their non-trivial topological phases. Off these three phases, we observed that, the α-phase of nine HH oxides (wherein the transition metal atoms occupy 4a Wyckoff positions in the crystal structure) is the most promising with non-trivial topological phase, governed by the Mass-Darwin relativistic effects which enhances the E_{BIS} function. Whereas the other phases are either trivial semi-conductors or conductors. We find that the E_{BIS} in the α-phase is as high as – 2.37 eV which would remain robust under ambient conditions. We also find that under modest strain fields, the band inversion strength is robust retaining the non-trivial character. The non-trivial character of these compounds is further verified by analyzing the orbital characters across the Fermi level, ARPES-like surface state spectra, slab band structures and the Z_2 invariants. We believe that the α-phase of HH oxides presented here can be synthesized experimentally for diverse room temperature applications.

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