## Search for novel topological Weyl semimetal phases

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Topology in various guises plays a central role in modern condensed matter physics. Although the original applications of topological ideas to band structures in semiconductors relied on the existence of a fully gapped bulk spectrum, more recently it has been recognized that protected surface states can arise even in gapless systems. The prototypical example of a gapless topological phase is a Weyl semi-metal showing linear dispersion around nodes termed as Weyl points, as the three-dimensional analog of graphene. Surface Fermi arcs are the most prominent manifestation of the topological nature of Weyl semi-metals. I will present predictions of the emergence of Weyl semimetal phase in two distinct cases:

(1)The topological crystalline insulator, Pb1xSnxTe exhibits topological phase transition upon the band inversion strength which can be tailored by the substitutional mixing ratio, strain, thermal expansion, ferroelectric displacement, and/or material thickness via quantum confinement effect. The SnTe building block of the compound is also known to exhibit a ferroelectric transition at low temperatures which leads to inversion symmetry breakdown. Using ab-initio-tight-binding calculations we have explored the parameter space associated with both band inversion and ferroelectric displacement. The calculated topological phase diagram shows the emergence of a Weyl semimetal phase which can be tuned with an external magnetic field [1].

(2)The interfacial phase-change memory (iPCM) GeTe/Sb2Te3 continues to attract a great deal of interest not only because they are promising candidates for the next generation non-volatile random-access memories but also for their fascinating topological properties. Depending on the atomic-layer-stacking sequence of the GeTe block the iPCM can be either in the “SET” (Ge-Te-Ge-Te) or “RESET” (Te-Ge-Ge-Te) states where the former exhibits a ferroelectric polarization and an electric conductivity which is two orders of magnitude higher than that of the RESET state. Ab initio electronic structure calculations reveal that the ferroelectric polarization in the ”SET” phase which breaks the inversion symmetry results in the emergence of a Weyl semimetal phase with a large electric conductivity due to the gapless Weyl nodes.

[l] T. Liang, et al., Science (May 2017)