Topological Materials

Hsin Lin[1,*]

[1]*Institute of Physics, Academia Sinica, Taipei 11529, Taiwan*

[*] E-mail: nilnish@gmail.com

Topological materials host various novel quantum phases of electrons which are characterized by band topology and topologically protected surface/edge states. [1] Despite recent progress, intense world-wide research activity in search of new classes of topological materials is continuing unabated. This interest is driven by the need for materials with greater structural flexibility and tunability to enable viable applications in spintronics and quantum computing. We have used first-principles band theory computations to successfully predict many new classes of 3D topologically interesting materials, including Bi_2Se_3 series, [2] the ternary half-Heusler compounds, [3] $TlBiSe_2$ family, [4] Li_2AgSb-class, and $GeBi_2Te_4$ family as well as topological crystalline insulator (TCI) SnTe family [5] and Weyl semimetals TaAs, [6,7] $SrSi_2$, [8] $(Mo,W)Te_2$, [9] Ta_3S_2, [10] and LaAlGe family. [11,12] I will also highlight our recent work on unconventional chiral fermions in RhSi, [13] cubic Dirac points in $LiOsO_3$, [14] and rotaional symmetry protected TCIs. [15] A brief discussion on Kramer-Weyl fermions in non-magnetic chiral cyrstals will be given. [16]

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