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Topological Materials

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Topological materials host various novel quantum phases of electrons which are characterized by band topology and topologically protected surface/edge states. 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 Bi₂Se₃ series, the ternary half-Heusler compounds, TlBiSe₂ family, Li₂AgSb-class, and GeBi₂Te₄ family as well as topological crystalline insulator (TCI) SnTe family and Weyl semimetals TaAs, SrSi₂, (Mo,W)Te₂, Ta₃S₂, and LaAlGe family. I will also highlight our recent work on 3D type-II Dirac semimetals in VA13 family.