Topological Semimetals and Weyl Fermions

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Topological semimetals, characterized by Weyl/Dirac nodes in the bulk and Fermi arcs on the surfaces, are new states of three-dimensional (3D) quantum matters, different from topological insulators. Weyl nodes are stable topological objects, and can be viewed as effective magnetic monopoles in the 3D momentum space. Its time-reversal invariant version ---- 3D Dirac node, however, consists of two copies of distinct Weyl nodes with opposite chirality, and requires additional symmetry protection, such as the crystal symmetry. Due to the presence of chiral anomaly, novel properties, such as negative magneto-resistance and non-local transport, can be expected for such semimetals. Recently, several Dirac semimetals (Na3Bi and Cd3As2) and Weyl semimetals (HgCr2Se4 and TaAs family) compounds have been predicted and experimentally verified. In this talk, I will review the theoretical progress with focus on the predictive roles of first-principles calculations in this field. Some recent experimental progress will be also addressed.