Dirac Semimetal in Three Dimensions

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In a Dirac semimetal, the conduction and valence bands contact only at discrete (Dirac) points in the Brillouin zone (BZ) and disperse linearly in all directions around these critical points. Including spin, the low energy effective theory around each critical point is a four band Dirac Hamiltonian. In two dimensions (2D), this situation is realized in graphene without spin-orbit coupling [1]. 3D Dirac points are predicted to exist at the phase transition between a topological and a normal insulator in the presence of inversion symmetry [2, 3]. Here we show that 3D Dirac points can also be protected by crystallographic symmetries in particular space-groups and enumerate the criteria necessary to identify these groups. This reveals the possibility of 3D analogs to graphene. We provide a systematic approach for identifying such materials and present ab initio calculations of metastable β-cristobalite BiO_2 which exhibits Dirac points at the three symmetry related X points of the BZ.

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