Dirac Point Degenerate with Massive Bands at a Topological Quantum Critical Point[1] SWAPNONIL BANERJEE, WARREN PICKETT, JUSTIN SMITH, VICTOR PARDO — In the band structure of the Skutterudite, as the Sb sublattice in the unit cell is moved slightly retaining the crystal symmetry, the small gap at the Fermi energy closes due to a band crossing at Gamma. At this critical point a pair of linear ("Dirac") bands are degenerate with two conventional bands. Because of the crystal symmetry three out of the four bands are degenerate even when one is away from the critical point. Insulators in 3D, as well as in 2D, can be characterized by topological invariants. When inversion symmetry is present (as in the space group 204 of Skutterudite), the Z2 invariant can be obtained from the parities of the occupied states at the invariant momenta, which in the bcc structure consist of Gamma, three H points, and the four P points. Here only the Gamma point requires consideration, since reoccupation occurs only there. The singlet has odd parity at Gamma while for the triplet it is even. As the critical point is crossed, the product of the parities of the occupied bands at Gamma, and hence the Z2 invariant, changes sign due to the reversal of the singlet- triplet position; the signal of a trivial to topological transition.

Swapnonil Banerjee
UC Davis, CA

Date submitted: 01 Oct 2010   Electronic form version 1.4