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Dirac semimetal to Weyl semimetal phase transition in strained Ca_3BiP

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Antiperovskite compounds with pnictide and alkaline earth elements, viz. Ca_3BiP are predicted to be narrow gap semiconductors with conduction band minimum and valence band maximum at the Γ point. Inclusion of spin-orbit coupling may invert the band ordering giving a non-trivial topological phase. Study of Ca_3BiP shows that compressive strain opens up a gap while maintaining the inverted band ordering, producing a topological insulator. Tensile strain, on the other hand, gaps everywhere except a single point along the direction of the strain, giving a Dirac semimetal, where the Dirac point is protected by the tetragonal symmetry. In this presentation, I will show that breaking the time-reversal symmetry gives rise to a type-I Weyl semimetal, using strained Ca_3BiP as an example, because the large SOC at the top of the valence bands makes it the most promising example. The position of the Weyl nodes in 3D Brillouin zone and the corresponding Weyl chirality will be described.