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Three-Dimensional Massive Dirac Fermion in the Bulk Band Structure of Cubic Inverse Perovskite Ca_3PbO

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— The band structure of a cubic inverse perovskite Ca_3PbO, which has been proposed as a candidate for a topological insulator, is analyzed by means of the first-principles calculation. It turns out that Ca3PbO is actually not a topological insulator, but a close observation of the calculated band structure near the Fermi energy reveals that there exist Dirac fermions in the bulk, instead of the surface, band structure. The Dirac fermion in this material is found on the Γ-X line in the momentum space and remarkably exactly at the Fermi energy in the energy space. It should also be noted that the discovered Dirac fermion is three-dimensional and massive with a very small mass of about 10^{-2} of the bare electron mass. The origin of the Dirac fermion in Ca_3PbO and the band structure of the materials related to Ca_3PbO will also be discussed.

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