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Topological Nodal Line Semimetals in CaP₃ family of materials

QIUNAN XU, Institute of Physics (IOP), Chinese Academy of Sciences (CAS), RUI YU, Harbin Institute of Technology, ZHONG FANG, XI DAI, HONGMING WENG, Institute of Physics (IOP), Chinese Academy of Sciences (CAS) — By using first-principle calculations and k-p model analysis, we propose that the three-dimensional (3D) topological nodal line semimetal state can be realized in CaP₃ family of materials, which include CaP₃, CaAs₃, SrP₃, SrAs₃ and BaAs₃, when spin-orbit coupling (SOC) is ignored. The closed topological nodal line near the Fermi energy is protected by time-reversal symmetry and spatial inversion symmetry. Moreover, a drumhead-like two-dimensional surface states are also obtained on the c-direction surface of these materials. When SOC is included, the nodal line will open a gap and becomes a strong topological insulator with (1;100) Z₂ indices.

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