Three-Dimensional Dirac Electrons in Antiperovskite Ca_3PbO

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Dirac materials have emerged as a prominent topic in condensed matter physics. They exhibit linear energy-momentum dispersion at finite points or along curves in k space. In the past decade, cubic antiperovskites have been suggested as potential source of such novel topological phases of matter as three-dimensional (3D) massive Dirac electrons, topological crystalline insulators (TCI), topological nodal line semimetals, and topological superconductors. The prototypical example is Ca_3PbO which was theoretically predicted to host 3D gapped Dirac electrons [1–3]. The Dirac states result from a band inversion of the Ca 3d and Pb 6p bands at the Γ point. To verify these predictions, we have conducted soft X-ray angle-resolved photoemission spectroscopy (SX-ARPES) and experimentally confirmed the presence of the Dirac-like dispersion along the Γ−X direction in the 3D Brillouin zone. Furthermore, chemical substitution of Bi for Pb effectively tuned the Fermi level of Ca_3PbO without fundamentally changing its Dirac-like band structure [4]. In addition to the spectroscopic studies, Shubnikov-de Haas (SdH) oscillation measurements on Bi-doped Ca_3PbO reveal the distinct features of Dirac fermions: linear magnetoresistance, light effective mass, and a nontrivial Berry phase shift [5]. Our studies demonstrate that the cubic antiperovskite family provides a promising platform for the exploration of 3D Dirac fermion systems. Finally, we will shortly report our current investigation of novel Dirac materials in a cubic antiperovskite nitride system.

References:

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