Highlights

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Intertwined Rashba, Dirac, and Weyl Fermions in Hexagonal Hyperferroelectric

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By means of density functional theory based calculations, we study the role of spin-orbit coupling in the new family of ABC hexagonal hyperferroelectrics, which spontaneously polarize even in the presence of an unscreened depolarization field. We unveil an extremely rich physics strongly linked to ferroelectric properties, ranging from the electric control of bulk Rashba effect to the existence of a three-dimensional topological insulator phase, with concomitant topological surface states even in the ultrathin film limit. Dirac cones are found to be strongly modulated by the ferroelectric switching, opening interesting perspectives, e.g., for domain engineering and control of topological p-n junctions . Topological interface states and bulk bandgap can be tuned by interfacing few layers of a topological hyperferroelectric with a normal ferroelectric. Finally, a Weyl semimetal phase can be achieved by alloying the topological hyperferroelectric in a diluite solution with a normal ferroelectric.

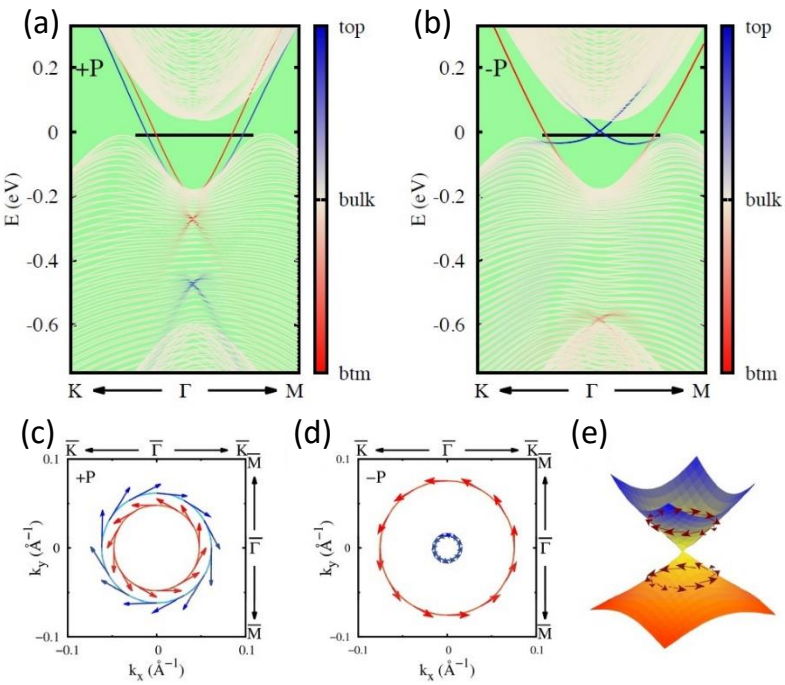

Figure 1. Surface states of KMgBi calculated in slab geometry for opposite direction of ferroelectric polarization, showing the strong tenability of Dirac cones arising from the interplay with ferroelectricity. Characters of top (MgBi-terminated) and bottom (K-terminated) surface states are highlighted by the color scale, revealing that the Dirac cones of K-terminated surfaces are always buried in the continuum of bulk states. (c), (d) display spin textures of the surface states at the energy cut shown in panels (a), (b), while (e) shows the reversal of spin-polarization chirality when crossing the Dirac cone.