

Engineering and probing topological properties of Dirac semimetal films by asymmetric charge transfer

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Dirac semimetals (DSMs) have topologically robust three-dimensional Dirac (doubled Weyl) nodes with Fermi-arc states. In heterostructures involving DSMs, charge transfer occurs at the interfaces, which can be used to probe and control their bulk and surface topological properties through surface-bulk connectivity. Here we demonstrate that despite a band gap in DSM films, asymmetric charge transfer at the surface enables one to accurately identify locations of the Dirac-node projections from gapless band crossings and to examine and engineer properties of the topological Fermi-arc surface states connecting the projections, by simulating adatom-adsorbed DSM films using a first-principles method with an effective model. The positions of the Dirac-node projections are insensitive to charge transfer amount or slab thickness except for extremely thin films. By varying the amount of charge transfer, unique spin textures near the projections and a separation between the Fermi-arc states change, which can be observed by gating without adatoms.