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Symmetry-Protected Dirac Semi-Metallic Phases in Transition Metal Dichalcogenides

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Abstract : Transition metal dichalcogenides have experienced a resurgence of interest in the past few years owing to their rich properties, ranging from metals and superconductors to strongly spin-orbit-coupled semiconductors and charge-density-wave systems. In all these cases, the transition metal d-electrons mainly determine the ground state properties. This presentation focuses on the chalcogen-derived states. Combining density-functional theory calculations with spin- and angle-resolved photoemission, it is shown that these states generically host a coexistence of type I and type II three-dimensional bulk Dirac fermions as well as ladders of topological surface states and surface resonances. It will be discussed how these naturally arise within a single p-orbital manifold as a general consequence of a trigonal crystal field, and as such can be expected across many compounds. Our finding opens a new route to design topological materials with advanced functionalities.

Keywords : topology, electronic structure, Dirac semimetals, transition metal dichalcogenides
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