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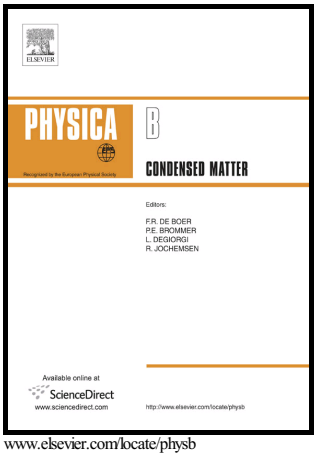

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Electronic band structure of 4*d* and 5*d* transition metal trichalcogenides

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Abstract

Transition metal trichalcogenides (TMTs), a family of van der Waals materials, have gained increasing interests from the discovery of magnetism in few-layer forms. Although TMTs with 3*d* transition metal elements have been studied extensively, much less is explored for the 4*d* and 5*d* cases, where the interesting interplay between electron correlations and the relativistic spin-orbit coupling is expected. Using *ab initio* calculations, we here investigate the electronic property of TMTs with 4*d* and 5*d* transition metal elements. We show that the band structures exhibit multiple node-like features near the Fermi level. These are the remnant of multiple Dirac cones that were recently discovered in the monolayer cases. Our results indicate that the peculiar two-dimensional multiple Dirac cones are concealed even in the layered bulk systems.

Keywords: van der Waals material, transition metal trichalcogenide, electronic band structure, spin-orbit coupling, Dirac electrons

1. Introduction

Magnetism in van der Waals (vdW) materials has drawn considerable attention owing to the possibility of two-dimensional magnetism in the quasi-two-dimensional structures. Amongst others transition metal trichalcogenides (TMTs), which have a layered structure of the honeycomb network of TM cations, have intensively studied as a promising candidate. Indeed, a variety of magnetic states were discovered in the bulk form of 3*d* TMTs, such as ferromagnetic, Néel, and zigzag antiferromagnetic states [1, 2, 3], and very recently, even in the atomically-thin form [4, 5, 6]. From the theoretical point of view, previous *ab initio* studies suggested the importance of strong electron correlations of 3*d* electrons in the