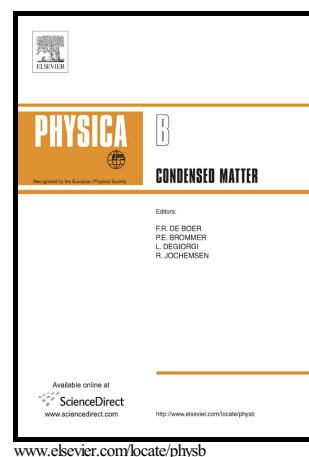


Electronic band structure of $4d$ and $5d$ transition metal trichalcogenides

Yusuke Sugita, Takashi Miyake, Yukitoshi Motome



PII: S0921-4526(17)30865-7
DOI: <https://doi.org/10.1016/j.physb.2017.10.126>
Reference: PHYSB310483

To appear in: *Physica B: Physics of Condensed Matter*

Received date: 30 June 2017

Accepted date: 31 October 2017

Cite this article as: Yusuke Sugita, Takashi Miyake and Yukitoshi Motome, Electronic band structure of $4d$ and $5d$ transition metal trichalcogenides, *Physica B: Physics of Condensed Matter*, <https://doi.org/10.1016/j.physb.2017.10.126>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting galley proof before it is published in its final citable form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

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

Yusuke Sugita^a, Takashi Miyake^b, and Yukitoshi Motome^a

^a*Department of Applied Physics, University of Tokyo, Bunkyo, Tokyo 113-8656, Japan*

^b*CD-FMat, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki 305-8568, Japan*

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 $3d$ transition metal elements have been studied extensively, much less is explored for the $4d$ and $5d$ 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 $4d$ and $5d$ 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 $3d$ 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 $3d$ electrons in the

Download English Version:

<https://daneshyari.com/en/article/8160883>

Download Persian Version:

<https://daneshyari.com/article/8160883>

[Daneshyari.com](https://daneshyari.com)