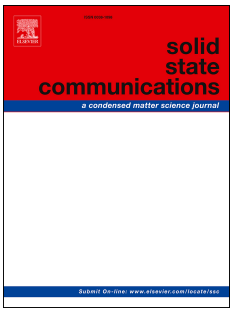
Accepted Manuscript



The structural, electronic and magnetic properties of CoS_2 under pressure

Zhong-Ying Feng, Yan Yang, Jian-Min Zhang

PII: S0038-1098(18)30059-0

DOI: 10.1016/j.ssc.2018.02.010

Reference: SSC 13388

To appear in: *Solid State Communications*

Received Date: 28 November 2017

Revised Date: 19 January 2018

Accepted Date: 12 February 2018

Please cite this article as: Z.-Y. Feng, Y. Yang, J.-M. Zhang, The structural, electronic and magnetic properties of CoS_2 under pressure, *Solid State Communications* (2018), doi: 10.1016/j.ssc.2018.02.010.

The structural, electronic and magnetic properties of CoS_2 under pressure

Zhong-Ying Feng [1, 2], Yan Yang [1, 3], Jian-Min Zhang [1, *]

1. *College of Physics and Information Technology, Shaanxi Normal University, Xian 710119, Shaanxi, PR China*

2. *Department of Science, Taiyuan Institute of Technology, Taiyuan 030008, Shanxi, PR China*

3. *Department of Physics, College of Science, North University of China, Taiyuan 030051, Shanxi, PR China*

A B S T R A C T

The structural, electronic and magnetic properties of CoS_2 under pressure have been investigated by the first-principles calculations. The lattice constant and volume decrease with increasing pressure. The CoS_2 is stable and behaves a brittle characteristic under the pressures of 0-5 GPa. The CoS_2 presents metallic characteristic under the pressures of 1-5 GPa although it is nearly half-metal (HM) under the pressure of 0 GPa. The lowest conduction bands for spin-up and spin-down channels shift towards higher and lower energy region, respectively, with the pressure increasing from 0 to 5 GPa. In spin-up channel the conduction band minimum (CBM) is mainly contributed by Co-3d(e_g) orbitals at R point but the valence band maximum (VBM) is contributed by Co-3d(t_{2g}) orbitals near M point. While in spin-down channel the CBM is contributed by S-3p orbitals at Γ point but the VBM is contributed by Co-3d(t_{2g}) orbitals near X point. The CoS_2 is still suitable to be used in the supercapacitor under the environmental pressures of 0-5 GPa due to the high conductivity.

Keywords: CoS_2; Structural property; Electronic property; Magnetic property; Pressure

1. Introduction

Supercapacitor has been paid widely attentions and has been applied in hydrid electric vehicles in recent years, due to the key role of energy storage device. As a typical pyrite-type transition-metal dichalcogenides and a great potential active material for supercapacitors, the itinerant electron ferromagnet CoS_2 with a Curie temperature $T_C \approx 120K$ [1] has been studied by plenty of researchers, due to large power density, high specific capacitance, and good cycling stability [2-6]. Besides, the half-metal (HM) materials with 100% spin-polarization at the Fermi level can be a good candidate to be used in the spintronic devices. Although the electronic and optical properties, as well as the magneto-optical Kerr effect in pyrite-structured CoS_2 have been studied by Saha *et al.* using first-principles methods, due to the possible half-metallic character which are of high technological importance [7], Wang *et al.* [8] and Brown *et al.* [9] have found the predicted HM character cannot be observed. The Co-e_g bands have been researched and different conclusions are found [10-12]. Antonov *et al.* have found that CoS_2 is almost a half-metallic ferromagnet with the

*Corresponding author. Tel.: +86 29 81530750.
E-mail address: jmzhang@snnu.edu.cn (J.-M. Zhang).