ASEC 2022

MDPI

Abstract

Band Gap Closure in MnS under Pressure †

Evgeniy Chernov [1,*] and Alexey Lukoyanov [2]

[1] M.N. Miheev Institute of Metal Physics of Ural Branch of Russian Academy of Sciences, 620108 Ekaterinburg, Russia
[2] Ural Federal University, Mira St. 19, 620002 Ekaterinburg, Russia; lukoyanov@imp.uran.ru
* Correspondence: chernov_ed@imp.uran.ru
† Presented at the 3rd International Electronic Conference on Applied Sciences, 1–15 December 2022; Available online: https://asec2022.sciforum.net/.

Citation: Chernov, E.; Lukoyanov, A. Band Gap Closure in MnS under Pressure. *Eng. Proc.* **2022**, *4*, x. https://doi.org/10.3390/xxxxx

Academic Editor(s):

Published: 1 December 2022

Abstract: Manganese chalcogenides are being actively studied both experimentally and theoretically because of metal-to-insulator transition under pressure and possible catalytic, optical and magnetic applications [1–3]. In particular, binary manganese sulphide MnS was found in several crystal phases: α–γ-MnS. The α-MnS phase crystallizes in cubic structure (Space Group $Fm\bar{3}m$), γ-MnS–in hexagonal structure (SG $P6_3mc$). It is known that γ-MnS is metastable when heated to 200–300 °C, it becomes the α-MnS phase [1]. We carried our theoretical studies of this compound taking into account antiferromagnetic ordering of the manganese ions at the ambient conditions and in compressed unit cells. To study the electronic structure of MnS, our calculations were done in the Quantum ESPRESSO software package [4] using the DFT + U method [5] for the Pedew-Burke-Ernsenhof (PBE) form of exchange-correlation functional [6]. MnS is a wide-band insulator in environmental conditions. In the course of the study, it was found out that in order to reproduce a wide gap, strong electronic correlations should be taken into account. Thus, to obtain the experimental value of the band gap, the values of the Coulomb interaction parameter U = 6.9 eV and the exchange interaction J = 0.86 eV were taken. It is also worth noting that taking into account electronic correlations affects the γ-MnS more strongly and when the maximum parameter of the Coulomb interaction parameter U = 6.9 eV is reached, the width of the electron gap of the γ-MnS reaches about 2 eV, while the α-MnS has a band gap width of no more than 1 eV. For compressed volumes of the unit cell, it was found that with increasing pressure on the unit cell, the band gap width decreases and finally closes for the cell volume, which is about 50% of the ambient volume. Thus, the closure of the energy gap and the increase in metallic states at Fermi energy demonstrate the experimentally observed transition from insulator to metal in the MnS.The work was supported by RFBR grant (project 20-02-00234).

Keywords: electronic structure; metal-insulator transition; strong electron correlations; dft

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