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Abstract

Band Gap Closure in MnS under Pressure †

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Manganese chalcogenides are being actively studied both experimentally and theoretically because of the metal-to-insulator transition under pressure and possible catalytic, optical and magnetic applications [1–3]. In particular, binary manganese sulfide MnS was found in several crystal phases: α–γ-MnS. The α-MnS phase crystallizes in cubic structure (Space Group $Fm\bar{3}m$), and 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 out our theoretical studies of this compound taking into account the 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 the exchange–correlation function [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 electron 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 electron 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 the Fermi energy demonstrate the experimentally observed transition from insulator to metal in MnS.

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