ELECTRONIC PROPERTIES OF QUASI-TWO-DIMENSIONAL MOLYBDENUM DISULFIDE WITH COBALT IMPURITIES

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Abstract – In variety of new materials a special place hold materials with nanoscale structure. Two-dimensional materials has attached a great attention due to its outstanding physical phenomena occurred at the nanolevel. There is a big interest in transition-metal dichalcogenides, due to their layered structure; they have extremely anisotropic properties, and therefore an intercalation processes easy to conduct. Reduced dimensionality can sometimes lead to magnetic behavior in systems, which are not magnetic in the bulk. That is why our investigation is aimed to determine the possibility of molybdenum disulfide (MoS_2) magnetic properties manifestation under cobalt (Co) impurities condition. Electronic properties study of quasi-two-dimensional structure of MoS_2 with Co impurities are presented. Calculations were carried out using VASP (Vienna *Ab initio* Simulation Package).

I. INTRODUCTION

Recent studies have demonstrated the important role of nanostructures in various fields of science and technology. Thus, molybdenum disulfide is a ‘‘layered’’ transition metal dichalcogenide semiconductor with an indirect band gap that has attracted considerable interest in connection with its catalytic and electronic properties [1]. The ‘‘layered’’ structure of MoS_2 (Fig. 1) is formed by a S–Mo–S sandwiches bonded together by weak Van-der-Waals forces (hexagonal unit cell parameters: a = 3,12 Å; b = 3,12 Å c =11,98 Å) [2]. The two-dimensional unit MoS_2 cell has one Mo atom and two S atoms. Each of the Mo atoms is coordinated to six S atoms in a triangular prismatic form. However, considering that Mo layer doesn’t lies in one plane with S layer it would be more correctly to conclude quasi-two-dimensional structure of MoS_2. Because of the weak van der Waals interactions between the sheets of sulfide atoms, MoS_2 has a low coefficient of friction, resulting in its lubricating properties. MoS_2 may be mechanically exfoliated using scotch tape to create 2D MoS_2 samples, similarly to graphene. MoS_2 has a number of unique properties, which allow it potential applications in transistors, flexible displays, and optics [3].

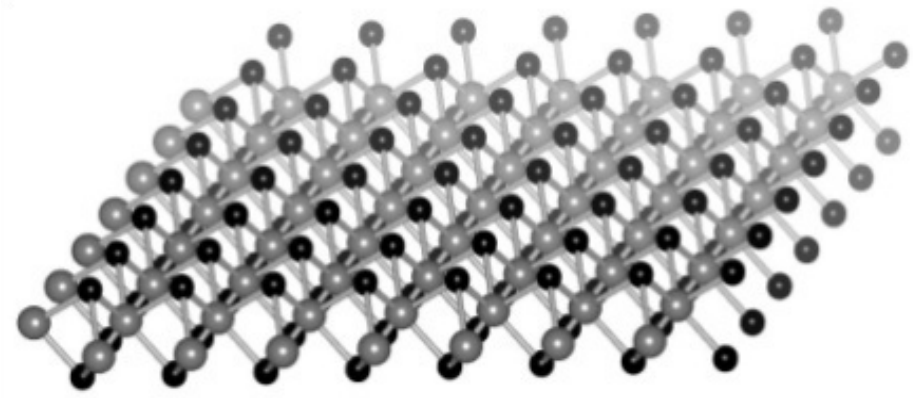


Figure 1 – Crystallographic structure of quasi-two-dimensional MoS_2

II. METHODOLOGY

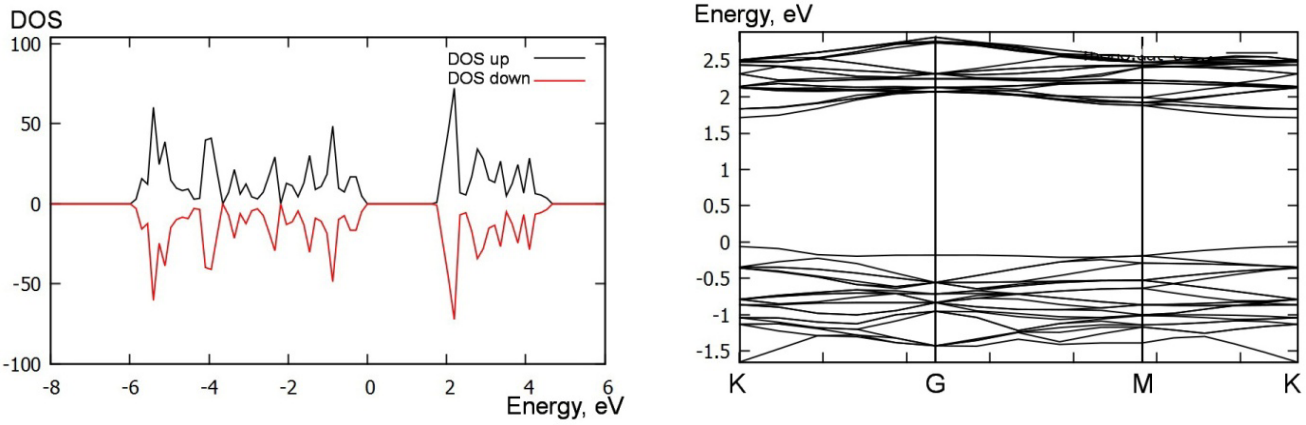
Nowadays a very important further step in electronic properties prediction is development of modern methods of materials simulation. Thus, further progress in understanding of physical phenomena at nanoscale level may be realized by use of *ab initio* simulations taking into account difficulties of experimental nanoobjects investigations.

A rather interesting problem is the investigation of nanostructured materials with impurities of magnetic metallic fragments, due to which manifestation of significant magnetic properties became possible as it was with the ternary compound $TlMeX_2$ [4].

The research presented in this paper aims to investigate the electronic and magnetic properties of quasi-two-dimensional molybdenum disulfide with impurities of cobalt, a well-known ferromagnetic metal. The study of spin-dependent properties of two-dimensional structure of MoS_2 with Co clusters impurities was carried out by means of a software package VASP (Vienna *Ab initio* Simulation Package) [5, 6]. The interaction between the ions and electrons in the simulated system is described by the Plane Augmented Waves (PAW) method. With the use of program package VASP it is possible to calculate the forces and stresses, which are used to relax atoms into their ground state. GGA-PBE pseudopotentials were applied for description of the interaction between the atomic cores and electrons. The calculations were performed using periodic conditions. In order to exclude the influence of impurities on each other a super-cell with size of 6 × 6 hexagonal unit cells of MoS_2 was created. Energy cutoff of 500 eV for the plane-wave expansion has been used.

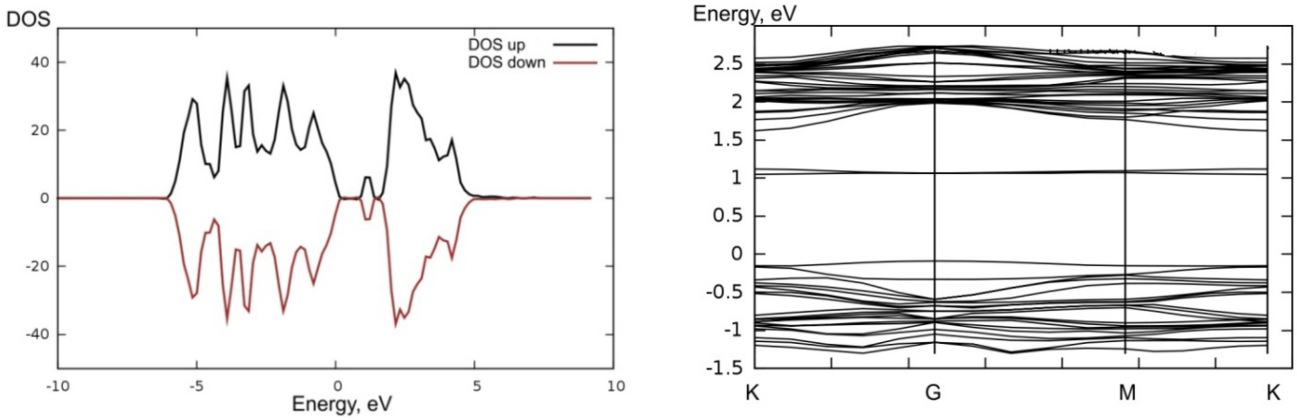
III. Results and Conclusion

Calculation results analysis of electronic density states and band diagram (Figs. 2, 3) of the perfect MoS_2 quasi-two-dimensional structure and MoS_2 structure with two Co-impurities shows the presence of additional energetic levels located near to band gap midpoint. Co impurity cluster increasing causes a sharp narrowing of the band gap to 0.91 eV and increasing of the magnetic moment value from 0.0008 μB (perfect quasi-two-dimensional structure) to 1.94 μB. Despite the observed changes of the electronic and magnetic properties with increasing impurity cluster, most of the MoS_2 structures still retain direct band transition. These facts suggest the possibility of using two-dimensional MoS_2 as a structural element for sensor and spintronic devices.



a) b)

Figure 2 – DOS (a) and energy bands (b) of the perfect quasi-two-dimensional MoS_2 structure



a) b)

Figure 3 – DOS (a) and energy bands (b) of quasi-two-dimensional MoS_2 structure with two Co-impurity clusters

Thus, within the framework of density functional theory using the software package VASP spin-dependent properties of quasi-two-dimensional MoS_2 structure with different size of Co impurity cluster were studied. Iit was shown a significant effect of Co impurity cluster on the electronic and magnetic properties of MoS_2. Further research in this area will allow to study in detail and explain the effect of impurities on the characteristics of investigated semiconductor.

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