

# Magnetic Ground State and Electronic Structure of Binary $Mn_2Sb$ Compound from Ab Initio Calculations <sup>†</sup>

Evgeniy D. Chernov <sup>1,2,\*</sup> and Alexey V. Lukoyanov <sup>2,1</sup>

<sup>1</sup> Ural Federal University Named after the First President of Russia B. N. Yeltsin, Ekaterinburg 620002, Russia; mr.cherjon@yandex.ru

<sup>2</sup> M.N. Miheev Institute of Metal Physics of Ural Branch of Russian Academy of Sciences, Ekaterinburg 620108, Russia; lukoyanov@imp.uran.ru

\* Correspondence: mr.cherjon@yandex.ru; Tel.: +0073433783886

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**Abstract:** Manganese antimonide  $Mn_{2-x}M_xSb$ , where  $M$  is a 3d transition metal, is a prominent binary material due to its high Curie temperature and magnetocaloric properties accompanying the  $M$ -induced first-order phase transition for various compositions. In this work we employed modern ab initio approach to analyze the magnetic ground state and electronic structure of  $Mn_2Sb$  for various types of long-range ordering. In the electronic structure of  $Mn_2Sb$ , it was found to possess the semi-metallic properties with a gap in the minority spin projection.

**Keywords:** electronic structure; ab initio methods; magnetic properties; magnetic ordering; ferrimagnetic ordering; total energy

## 1. Introduction

Binary manganese antimonide  $Mn_{2-x}M_xSb$  doped with transition metal  $M$ , is a promising material for spintronics due to its unique magnetic properties for various compositions. In addition to external factors (temperature, pressure, electric and magnetic fields) [1,2], the properties of binary compounds depend significantly on their crystal structure and composition [3–5]. The aim of this work is to analyze the electronic structure and magnetic properties of  $Mn_2Sb$  for various types of long-range ordering of the Mn magnetic moments.

## 2. Method

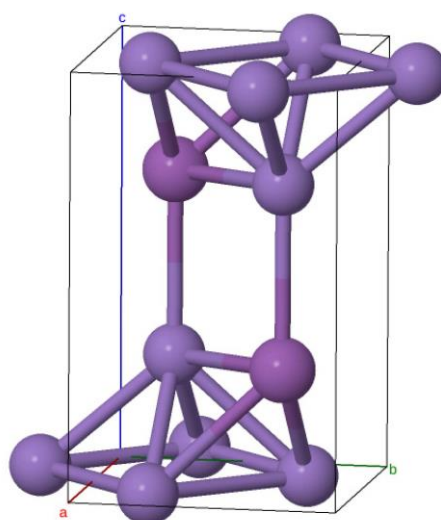
Our calculations of the electronic structure of the  $Mn_2Sb$  compound were performed in the TB-LMTO-ASA software package [6] based on method of linearized muffin-tin (MT) orbitals and the approximation of atomic spheres (ASA) with tight-binding approach (TB). This computational package implements local spin density approximation. The orbital basis included MT orbitals corresponding to the 4s-, 4p-, and 3d states of Mn and the 5s-, and 5p- electronic states of the Sb ions. The following radii of MT spheres were used in calculations: for Mn1—2.69 a. u., for Mn2—2.73 a. u., for Sb—3.46 a. u. The ab initio approach is based on the usage of experimental data on crystal structure only with no further fitting parameters from magnetic and other results. This theoretical approach allows one to model various types of magnetic ordering, spin-orbit coupling, applied pressure effects, magnetic field, and other external factors to improve the magnetic and spectral characteristics of materials.

### 3. Results

The  $Mn_2Sb$  compound has a tetragonal structure with the 129th space group ( $P4/nmm$ ) [7] (Table 1). The Mn atoms are located at two symmetrically independent crystallographic sites: Mn1 (point symmetry:  $4mm$ ) and Mn2 (point symmetry:  $-4m2$ ). The unit cell contains two crystallographically distinct sites of Mn1 and Mn2, which are respectively surrounded tetrahedrally and octahedrally by the Sb atoms. The ferrimagnetic structure is formed by an antiparallel arrangement of magnetic moments. The crystal structure is shown in Figure 1. The structure is stable over a wide temperature range, with the magnetic structure passing through a series of phase transitions. The magnetic phase transition in  $Mn_2Sb$  occurs at the Curie temperature  $T_c$  equal to 550 K [7]. Below this temperature, a ferrimagnetic ordering with unequal magnetic moments of different types of manganese ions is realized in the compound.

**Table 1.** Arrangement of  $Mn_2Sb$  atoms in the crystal lattice [7].

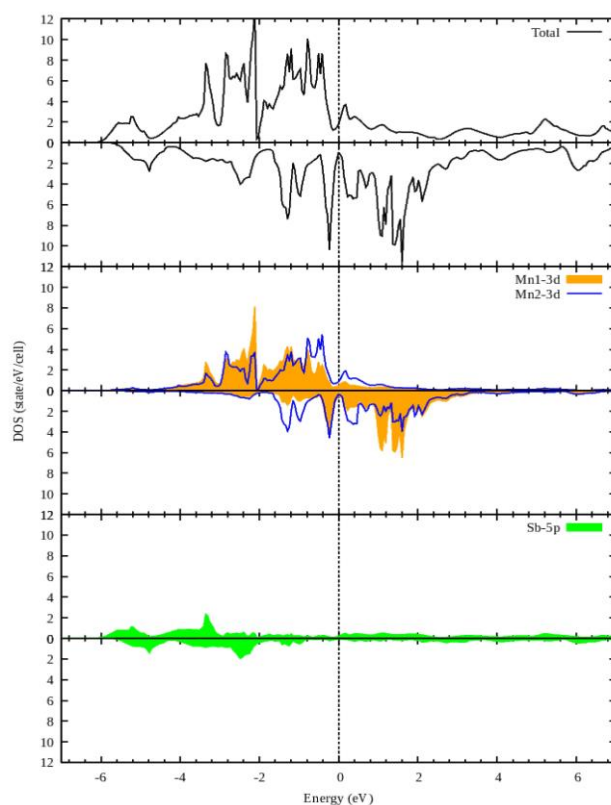
Ion	Wyckoff Symbol	Symmetry	X	Y	Z
Mn1	2c	$4mm$	1/4	1/4	0.27
Mn2	2a	$-4m2$	3/4	1/4	0
Sb	2c	$4mm$	1/4	1/4	0.7



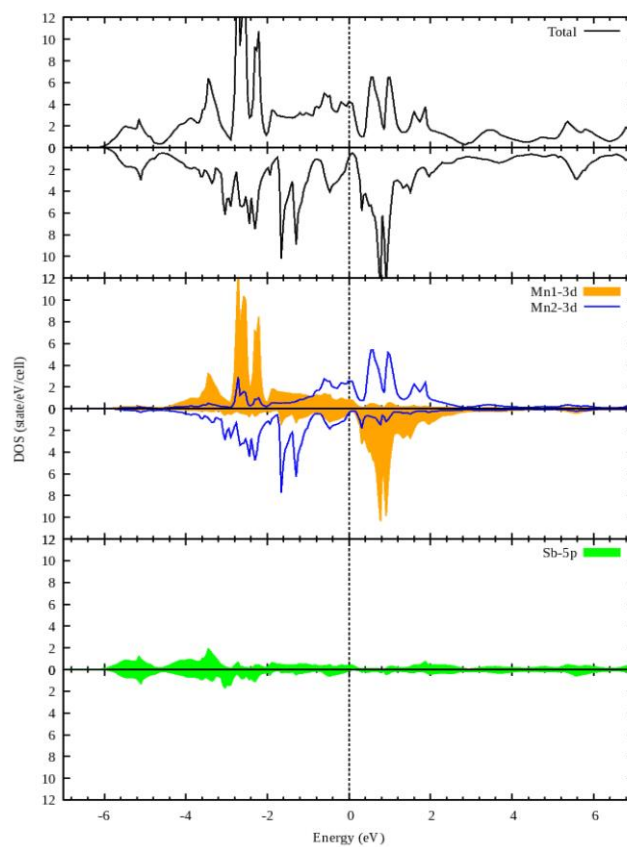
**Figure 1.** Crystal structure of the  $Mn_2Sb$  compound [7].

The density of electronic states in Figures 2 and 3 show that in the case of ferromagnetic and antiferromagnetic arrangement of manganese ions, the  $Mn_2Sb$  compound has metallic properties and passes a current with only one spin projection, majority. The figures are plotted relative to the Fermi level (indicated by a vertical dotted line).

In the case of calculations with the ferromagnetic ordering of the magnetic moments of the manganese ions, the magnetic moment for Mn1 was found to be 3.22 Bohr magnetons, and for Mn2 found to be equal to 2 Bohr magnetons, these values are close to the experimental ones: 2.13 and 3.87 Bohr magnetons [7]. In the case of the antiferromagnetic arrangement of the magnetic moments of the manganese ions, the magnetic moment for Mn1 was  $-3.47$  Bohr magnetons, and for Mn2 2.25 Bohr magnetons, which characterizes the  $Mn_2Sb$  compound as a ferrimagnet rather than an antiferromagnet, which is in good agreement with the previous results of calculations [7]. The total energy value in the case of ferromagnetic ordering was  $-35163.246$  Ry, and in the case of ferrimagnetic ordering of manganese ions  $-35163.274$  Ry. It follows that the ferrimagnetic ordering is more energetically preferable for the  $Mn_2Sb$  compounds.



**Figure 2.** Energy distribution of the density of electronic states calculated for Mn<sub>2</sub>Sb in the case of the ferromagnetic ordering of Mn.



**Figure 3.** Energy distribution of the density of electronic states calculated for Mn<sub>2</sub>Sb in the case of the ferrimagnetic ordering of Mn.

#### 4. Conclusions

Mn<sub>2</sub>Sb has a tetragonal type crystal structure. The unit cell contains two magnetic types of sites Mn1 and Mn2, tetrahedrally and octahedrally surrounded by Sb atoms, respectively. The structure is stable over a wide temperature range, with the magnetic structure passing through a series of phase transitions. As a result of calculations of the electronic structure of the Mn<sub>2</sub>Sb compound, it was found that this compound is a semi-metal, since it passes a current with only one spin projection. When comparing the total energies, it was found that the ferrimagnetic ordering of the magnetic moments of the manganese ions would be more energetically preferable. The ferrimagnetic structure is formed by an antiparallel arrangement of magnetic moments with different magnitude of the Mn magnetic moments and found to have the lowest total energy. We obtained the Mn magnetic moments as approximately −3.5 and 2.3 Bohr magnetons in a good agreement with experimental data. In the electronic structure of Mn<sub>2</sub>Sb, it was found to possess the semi-metallic properties with a gap in the minority spin projection.

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**Conflicts of Interest:** The authors declare no conflicts of interest.

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