Ural Federal University named after the first President of Russia B. N. Yeltsin, Ekaterinburg, Russia; M.N. Miheev Institute of Metal Physics of Ural Branch of Russian Academy of Sciences, Ekaterinburg, Russia

Magnetic ground state and electronic structure of binary Mn_2Sb compound from ab initio calculations

Evgeniy D. Chernov and Alexey V. Lukoyanov

mr.cherjon@yandex.ru and lukoyanov@imp.uran.ru

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Crystal structure

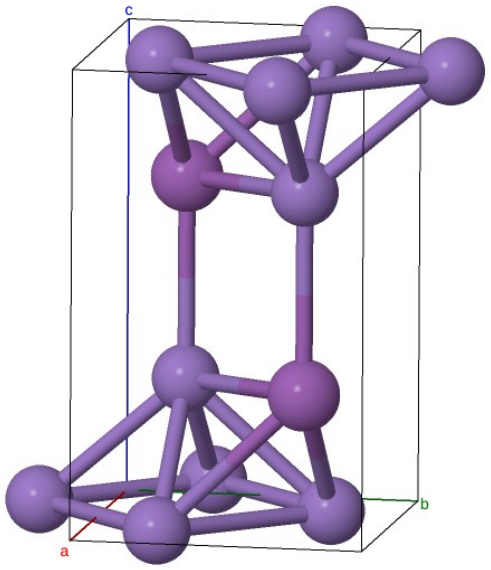

Figure 1. Crystal structure of the Mn2Sb compound.

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

Ion	Wycoff 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

We used TB-LMTO-ASA computational package

[1] Kanomata, T.; Ido, H. J. Appl. Phys. 1984, 55, 2039.

Electronic structure 1

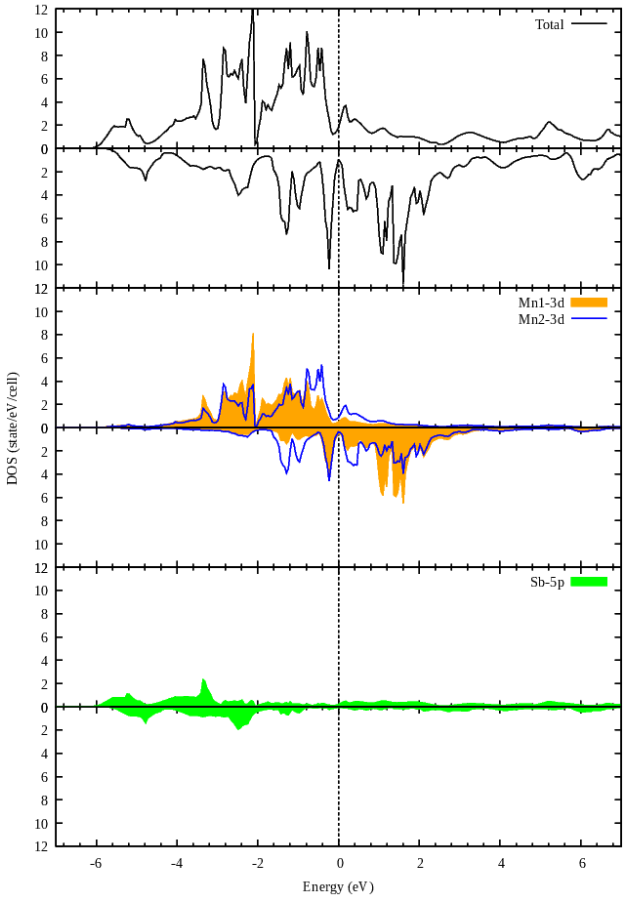

Figure 2. Energy distribution of the density of electronic states calculated for Mn_2Sb in the case of the **ferromagnetic** ordering.

Electronic structure 2

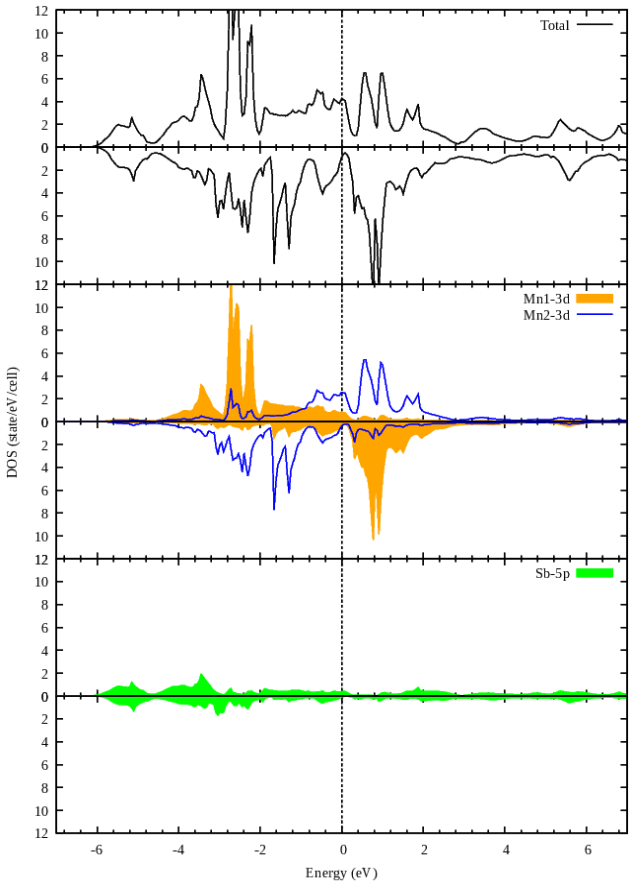

Figure 3. Energy distribution of the density of electronic States calculated for Mn_2Sb in the case of the **ferrimagnetic** ordering.

Conclusions

As a result of calculations of the electronic structure of the Mn_2Sb 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_2Sb, it was found to possess the semi-metallic properties with a gap in the minority spin projection.

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