M. N. Mikheev Institute of Metal Physics
of Ural Branch of Russian Academy of Sciences

The electronic structure and magnetic properties of full Heusler alloy Mn_2CrAl

Chernov E.D.[1], Filanovich A.N.[1,2], Lukoyanov A.V.[1,2]

[1]M.N. Mikheev Institute of Metal Physics, UrB of RAS,
Ekaterinburg, Russia
[2]Ural Federal University named aft. B.N. Eltsin, Ekaterinburg, Russia
*chernov_ed@imp.uran.ru

ASEC 2023
The 4th International Electronic Conference on Applied Sciences
27 October – 10 November 2023 | Online

➢ Introduction

ASEC 2023
The 4th International Electronic Conference on Applied Sciences
27 October – 10 November 2023 | Online

- The full Heusler alloys Mn_2MeZ, where Me is a 3d transition metal and Z – an element of group III–V, attract the attention of researchers as materials promising for magnetoelectronic and thermoelectric applications [1].
- These alloys may exhibit strong ferromagnetism or compensated ferrimagnetism up to high temperatures, phase transitions are possible in which the magnetic structure changes [2].
- The experiments for the Mn_2YAl systems (Y = Cr, Mn, Fe) demonstrate zero or close to it total magnetization that can be indicative of a compensated anti- or ferrimagnetism [2].
- This work is based on the results of calculations of the electronic structure and magnetic properties of two different phases of the Heusler alloy Mn_2CrAl.

*[1] C.Felser et al., APL Mater. **3**, 041518 (2015).*
*[2] V.V.Marchenkov et al., JETP **155**, 1083 (2019).*

➢ Computational approach

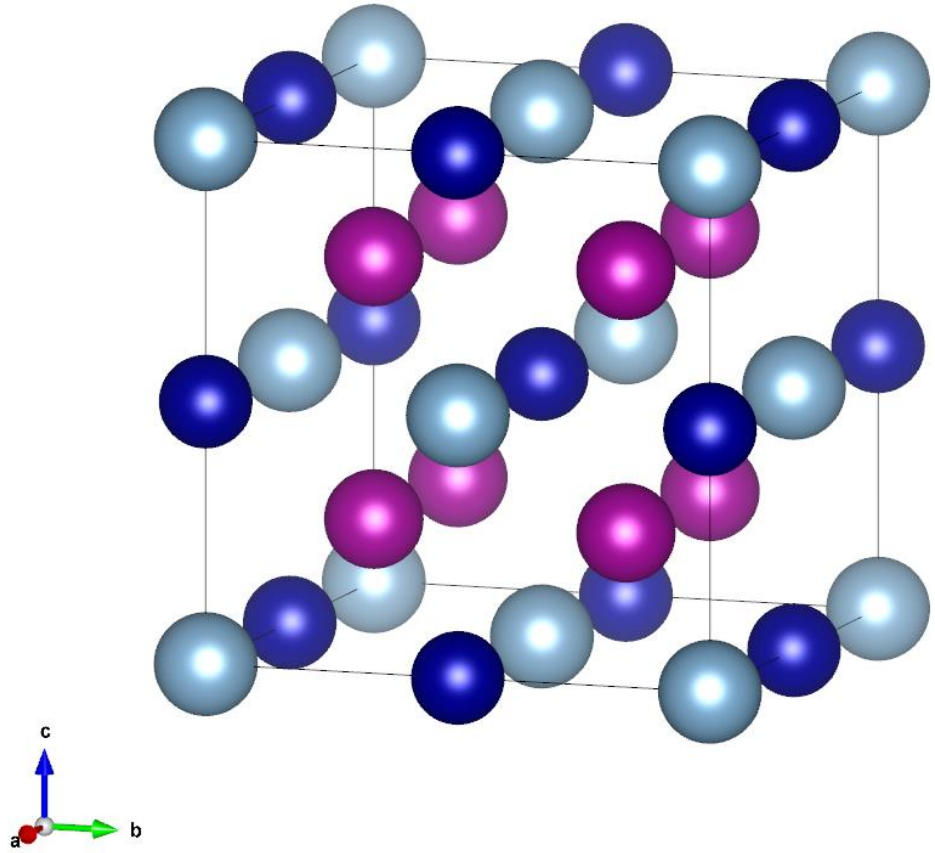
ASEC 2023
The 4th International Electronic Conference on Applied Sciences
27 October – 10 November 2023 | Online

- Density functional theory
- Generalize gradient appromixation
- Pseudopotential type is PBEsol (Perdew-Burke-Enzerhof) [3]
- DFT+U is using to account for electron correlation effects [4]. Used software package: Quantum Espresso [5]

[3] Perdew J.P. et al., Phys. Rev. Lett. 9, 767 (1996)
[4] Anisimov V.I., Gunnarsson O., Physical Review B 43, 7570-7574 (1991)
[5] Giannozzi P. et al., J. Phys.: Condens. Matter. 29, 465901 (2017)

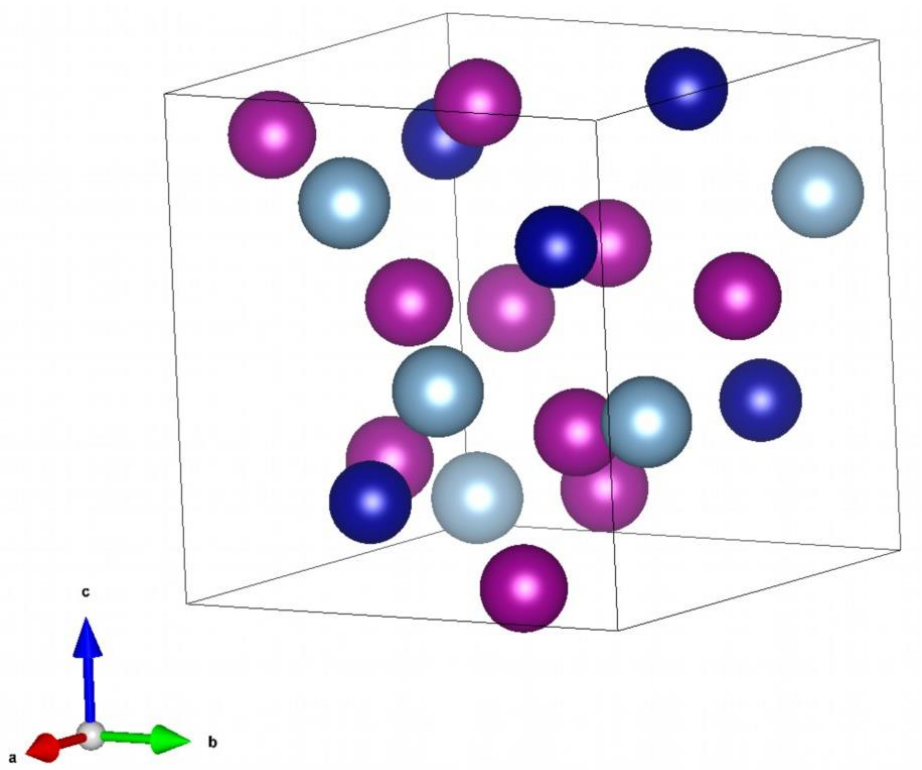
➢ Crystal structure of the $L2_1$-phase

- Structure: Cubic
- Space group number: 225
- Lattice parameter: 5.835 Å
- Atomic positions:
- Mn1 (-0.25, -0.25, -0.25)
- Mn2 (0.25, 0.25, 0.25)
- Cr (0.50, 0.50, 0.50)
- Al (0.00, 0.00, 0.00)



➢ Crystal structure of the β-Mn-phase

- Structure: Cubic
- Space group number: 213
- Lattice parameter: 6.408 Å



Atomic positions:			
Al	0.0636	0.0636	0.0636
Cr	0.3136	0.1864	-0.1864
Cr	-0.1864	0.3136	0.1864
Cr	0.1864	-0.1864	0.3136
Cr	-0.3136	-0.3136	-0.3136
Mn1	-0.4364	0.4364	-0.0636
Mn1	0.4364	-0.0636	-0.4364
Al	-0.0636	-0.4364	0.4364
Mn2	-0.2978	0.0478	-0.1250
Mn2	-0.1250	-0.2978	0.0478
Al	0.0478	-0.1250	-0.2978
Cr	0.3750	-0.2022	-0.0478
Al	-0.0478	0.3750	-0.2022
Al	-0.2022	-0.0478	0.3750
Mn2	0.4522	0.1250	0.2022
Mn2	0.2022	0.4522	0.1250
Mn2	0.1250	0.2022	0.4522
Mn2	-0.4522	-0.3750	0.2978
Mn2	0.2978	-0.4522	-0.3750
Mn2	-0.3750	0.2978	-0.4522

➢ Electronic structure of Mn_2CrAl (GGA)

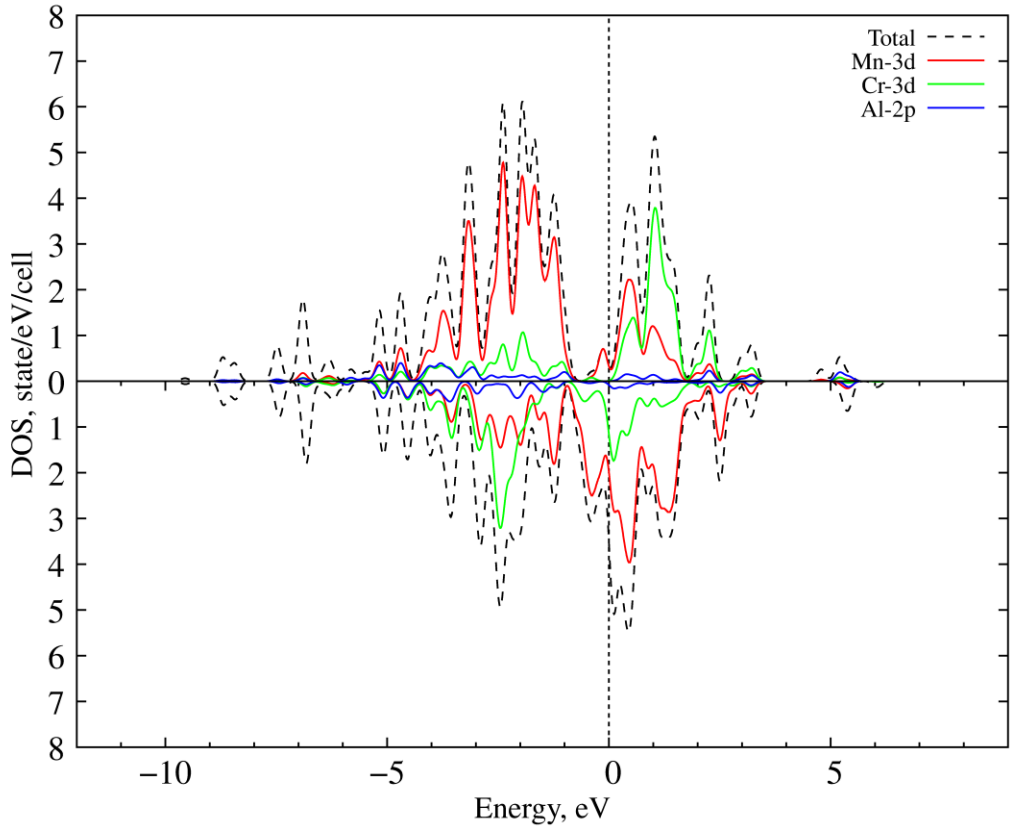


Fig. 1 The density of the states of the $L2_1$-type Mn_2CrAl in the GGA. The Fermi level is shifted to zero (a vertical dotted line).

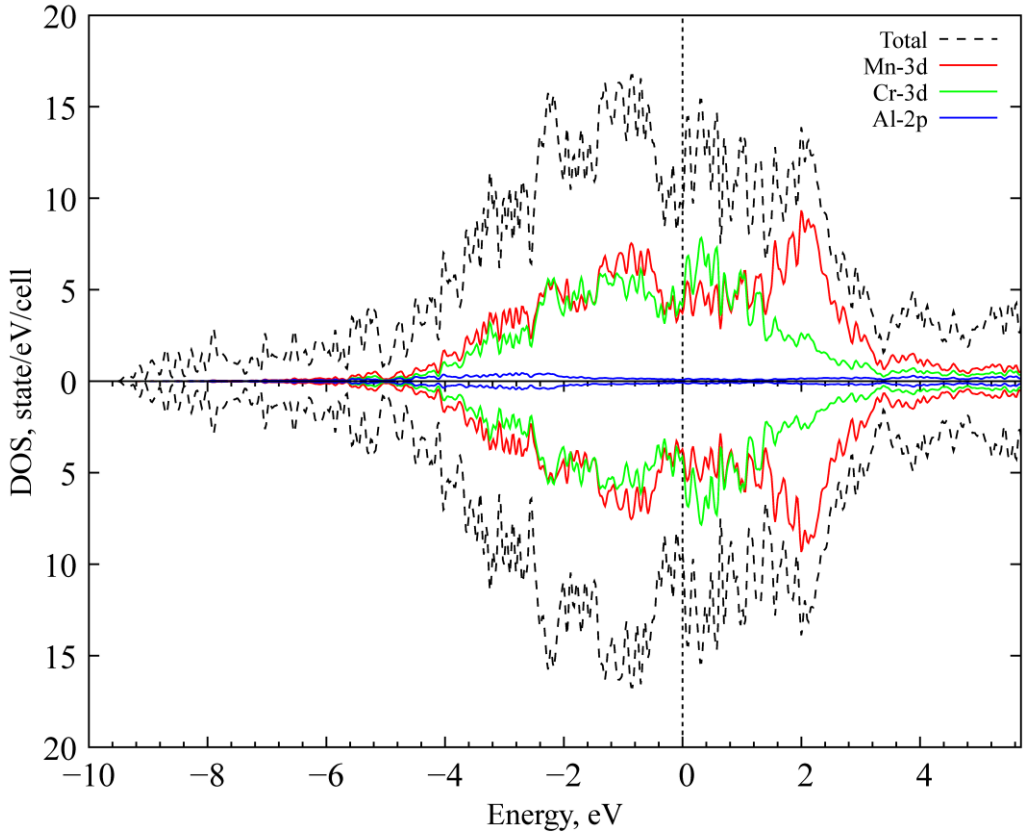


Fig. 2 The density of the states of the β-Mn-type Mn_2CrAl in GGA.

➢ Density of states of Mn_2CrAl in the case of accounting for electron correlation (U = 1 eV)

- The compound exhibits metallic properties.
- The localized Mn states peaks in the valance band shift to lower energies and in the conduction band to higher energies.
- Most Mn 3d states are observed in the valence band between -5 and -2 eV energies and in the conduction band between 0 and 4 eV energies.

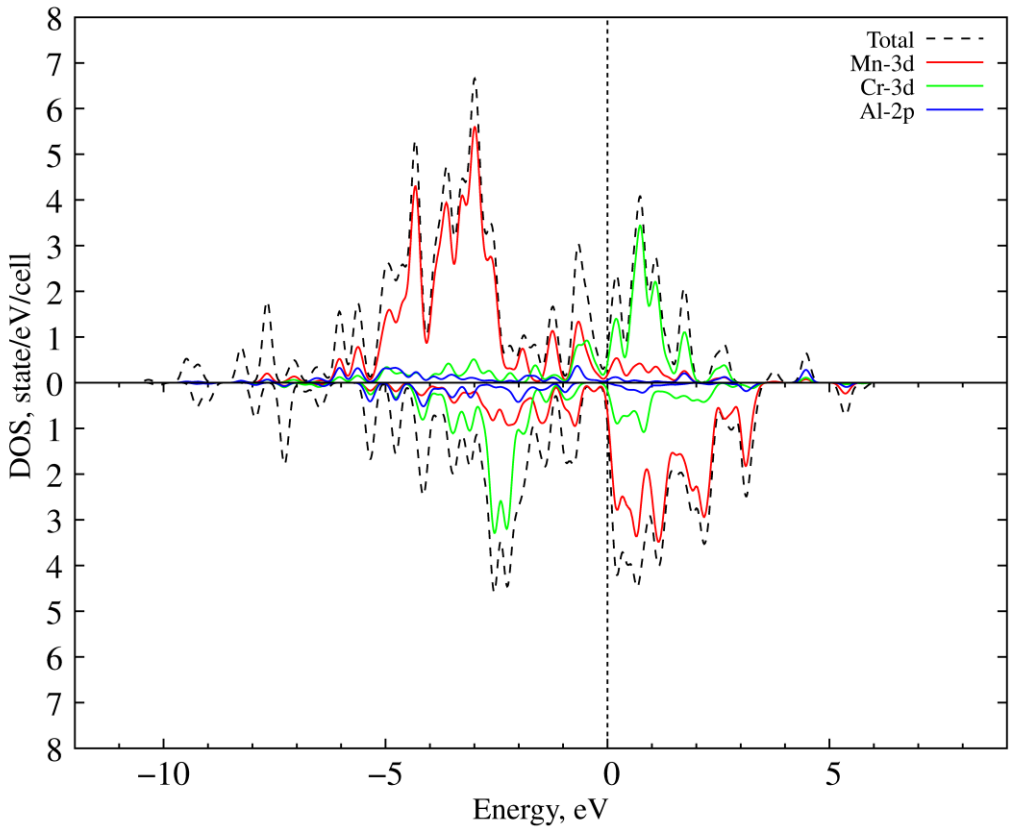


Fig. 3 The partial density of the states of Mn_2CrAl with U = 1 eV.

➢ Density of states of Mn_2CrAl in the case of accounting for electron correlation (U = 3 eV)

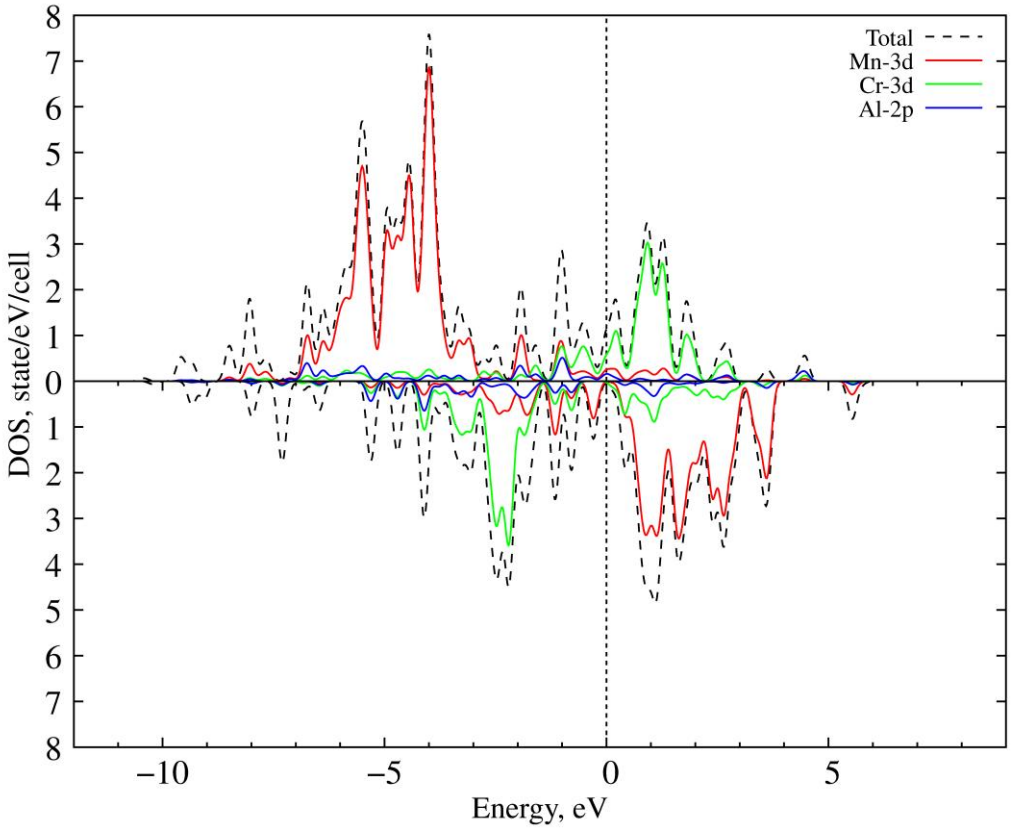


Fig. 4 The partial density of the states of Mn_2CrAl with U = 3 eV.

- The intensity of peaks of Mn increases.
- The distance between peaks of Mn states in the valance band and the conduction band increases with increasing of Coulomb parameter.
- The 3d Cr states are localized in valance band for the “majority” spin projection at -2.3 eV energy and at 1 eV energy in conduction band for the “majority” spin projection.

➢ Density of states of Mn_2CrAl in the case of accounting for electron correlation (U = 6 eV)

- Most of the manganese states have completely shifted towards lower energies in the valence band and towards higher energies in the conduction band
- The peaks of Mn states localize between -10 and -6 eV energies in the valence band and between 1 and 5 eV energies in the conduction band.
- The peaks of Cr states are not shifted.
- Mn_2CrAl still exhibits metallic properties.

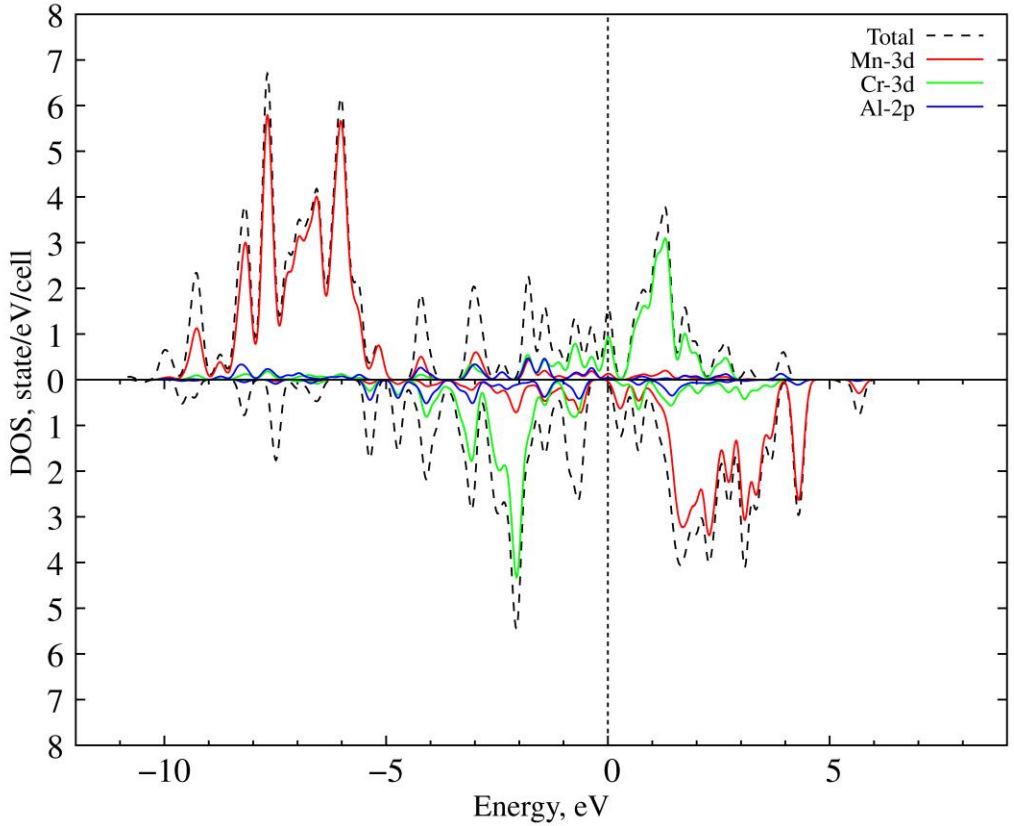


Fig. 5 The partial density of the states of Mn_2CrAl with the U = 6 eV.

➢ Magnetic properties of Mn_2CrAl

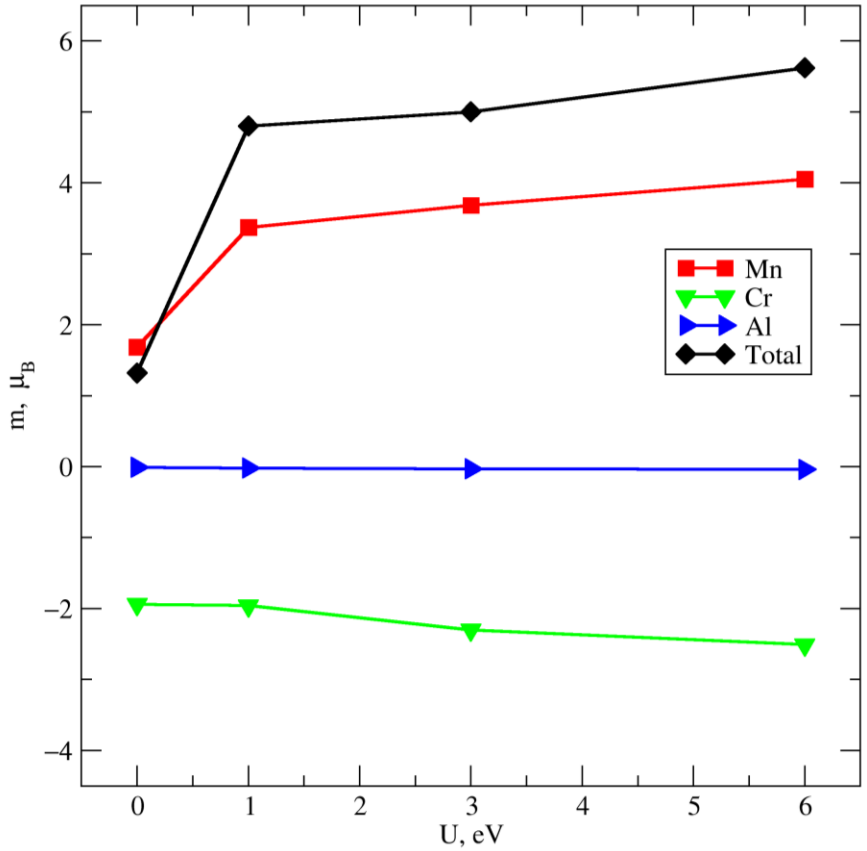


Fig. 6 The total and partial per ion magnetic moments for the L21-type Mn_2CrAl alloy for different values of the Coulomb interaction parameter.

Table 1. The magnetic moments per an ion in the L21-type Mn_2CrAl material depending on the U parameter value.

	Mn1, μ_B	Mn2, μ_B	Cr, μ_B	Al, μ_B	Tot, μ_B
GGA	1.68	1.68	-1.94	-0.01	1.32
U = 1 eV	3.37	3.37	-1.96	-0.02	4.80
U = 3 eV	3.68	3.68	-2.30	-0.03	5.00
U = 6 eV	4.05	4.05	-2.51	-0.04	5.62

➢ Conclusions

ASEC 2023 The 4th International Electronic Conference on Applied Sciences
27 October – 10 November 2023 | Online

- It was found that the electronic structure of Mn_2CrAl is metallic similar to Mn_2NiAl, and has a ferrimagnetic ordering of manganese ions. The electron correlations taken into account in GGA+U are demonstrated to increase the total moment in Mn_2CrAl.
- The β-Mn-type phase of Mn_2CrAl also exhibits ferrimagnetic properties with the total magnetic moment of 0.12 μ_B/f.u. which is in agreement with the experimental magnetization measurements.

This research was supported by the Russian Science Foundation, project no. 22-22-20109.

The results are published in:

1) Chernov, E.D.; Lukoyanov, A.V. *Magnetochemistry* 9, 185 (2023).
2) Shreder, E.I.; Filanovich A.N.; Chernov E.D.; et. al. *Phys. Met. Metallogr. 7*, 124 (2023).

M. N. Mikheev Institute of Metal Physics
of Ural Branch of Russian Academy of Sciences

Thank you for your attention!

ASEC 2023

The 4th International Electronic Conference on Applied Sciences

27 October – 10 November 2023 | Online