Exercise I: NiO

1) A Ni atom has the electronic configuration $[Ar]3d^8 4s^2$. In NiO, the nickel ions give away two s-electrons and have the valence state Ni^{2+}. Using Hund's rules, find the total spin S and the total orbital moment L of a Ni^{2+} ion.

2) Calculate the spin magnetic moment per Ni atom as $\mu_{Ni} = \gamma_s * S * \mu_B$, where $\gamma_s = 2$ is the spin gyromagnetic ratio.

Note: In crystalline materials, the orbital magnetic moment is usually much smaller that the spin magnetic moment due to orbital moment quenching. Therefore, we neglect the orbital magnetic moment in this exercise.

3) Compare the μ_{Ni} with the experimental value $1.70\mu_B$.
[https://www.vasp.at/wiki/index.php/NiO].

Exercise II: Fe

1) A Fe atom has the electronic configuration $[Ar]3d^6 4s^2$. Using the Hund's rules, calculate the spin magnetic moment of Fe atoms in a crystal in the framework of the atomic model $\mu_{Fe} = \gamma_s S \mu_B$. Compare the result with an experimental value of $2.15\mu_B$.

2) Calculate the DOS of bcc-Fe using MStudio.

a) Upload the Fe file from the database "3dMetals → Fe".

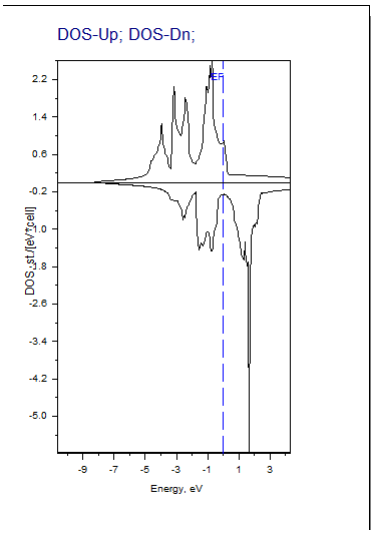
b) Do the self-consistent calculation checking for the convergence. If the convergence has not been reached, increase the limit of self-consistent loops.

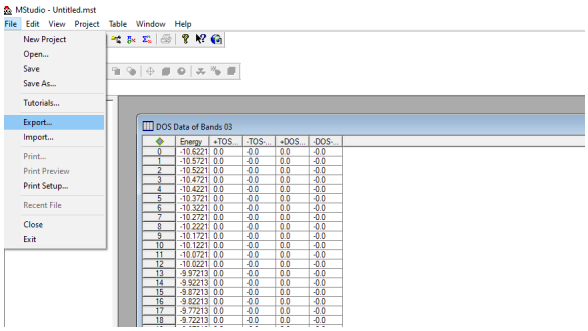
c) Calculate the DOS using the following parameters: Emin = 0 eV, Emax = 15 eV, number of points = 300, mesh = 15,15,15.

d) Export the DOS table to a .dat file using "File → Export..."

e) Upload the exported .dat file to Excel. Find the magnetic moment per Fe atom by integrating the last two columns (+DOS-up and -DOS-dn) using the following formula:

$$\mu_{Fe} = (n_\uparrow - n_\downarrow)\mu_B \tag{1}$$





$$n_{\uparrow} = 5 * \frac{\int_{filled\ states} dE\ DOS(spin\ up)}{\int dE\ DOS(spin\ up)} \tag{2}$$

$$n_{\downarrow} = 5 * \frac{\int_{filled\ states} dE\ DOS(spin\ down)}{\int dE\ DOS(spin\ down)} \tag{3}$$

Exercise III: Itinerant vs atomic magnetism

What is the difference between itinerant magnetism and atomic magnetism? Which materials can be better described by the itinerant model and which by the atomic?