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Getting started with FPLO-6: Basic handling of fedit

I. Default settings (e.g., numerical grids) are normally not touched by the user and need not be reported, since they are defined by the version number.

II. Technical settings (e.g., the chosen iteration scheme) may influence the calculation but do normally not change the result and are thus usually not reported.

III. Settings, that influence the result (e.g., Wyckoff positions, lattice parameters, number of k points, type of xc approximation) should always be reported. This also holds for any changes of the default numerical settings.

If you observe the last point you document a **reproducable computer experiment**.

mkdir Al-test

[pay attention to a tidy organization of your directories]

cd Al-test

fedit -h | more

fedit

[set up the input for the first calculation]

fplo > out

[run the first calculation]

ls

gv bravais.ps

gv primitive.ps

cd ..

grit Al

[check the sequence of iterations in Al*/out]

grEE Al

[check the final total energy in Al*/out]

```
cd -
view out
fedit -bandplot
```

[look at the band structure]

```
xmgrace +dos.total
```

[look at the density of states]

For the tasks, go to **hapu** and use:

bsub < **my_sub**

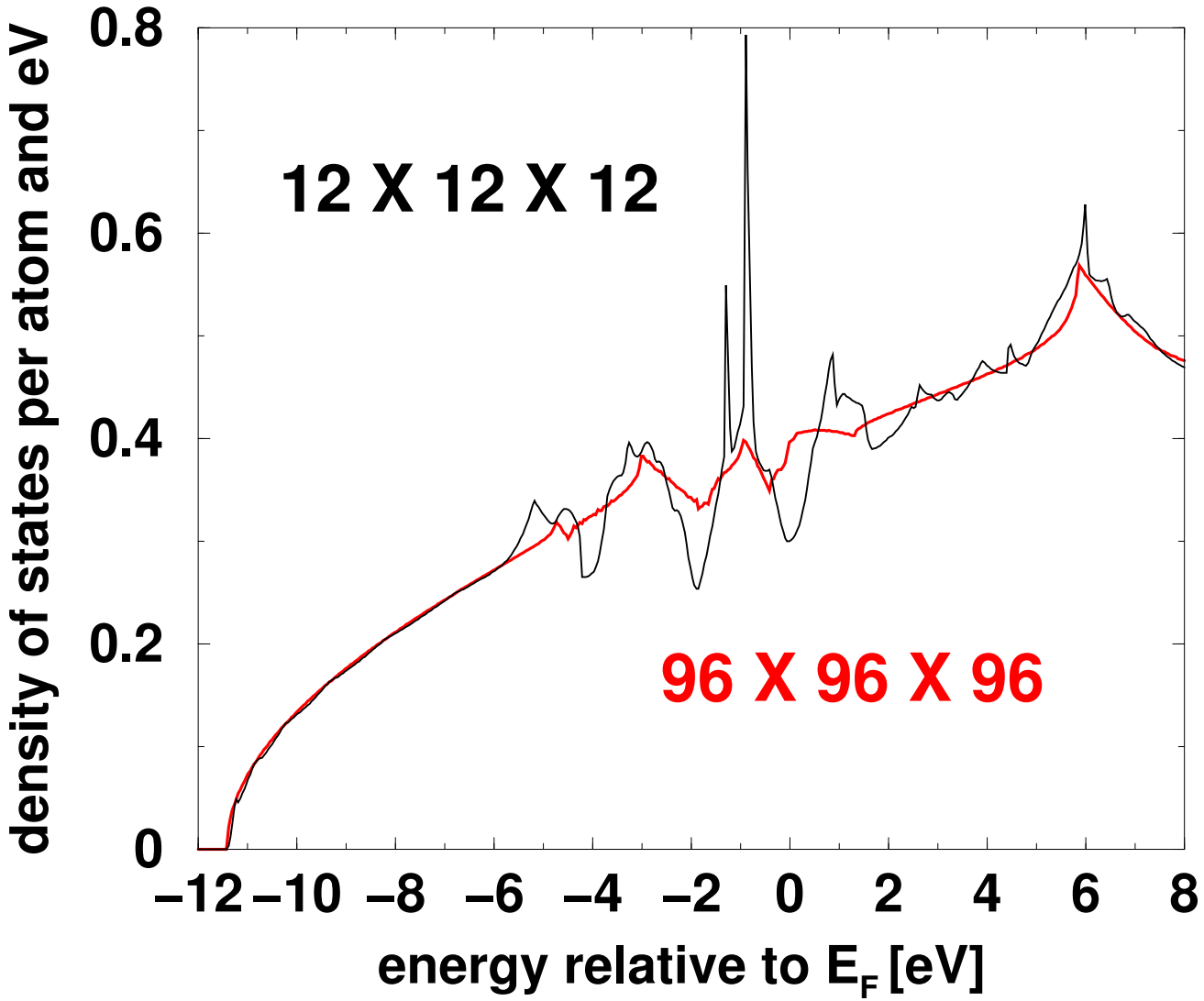
Do not run fplo > out on the hapu master.

Aluminum

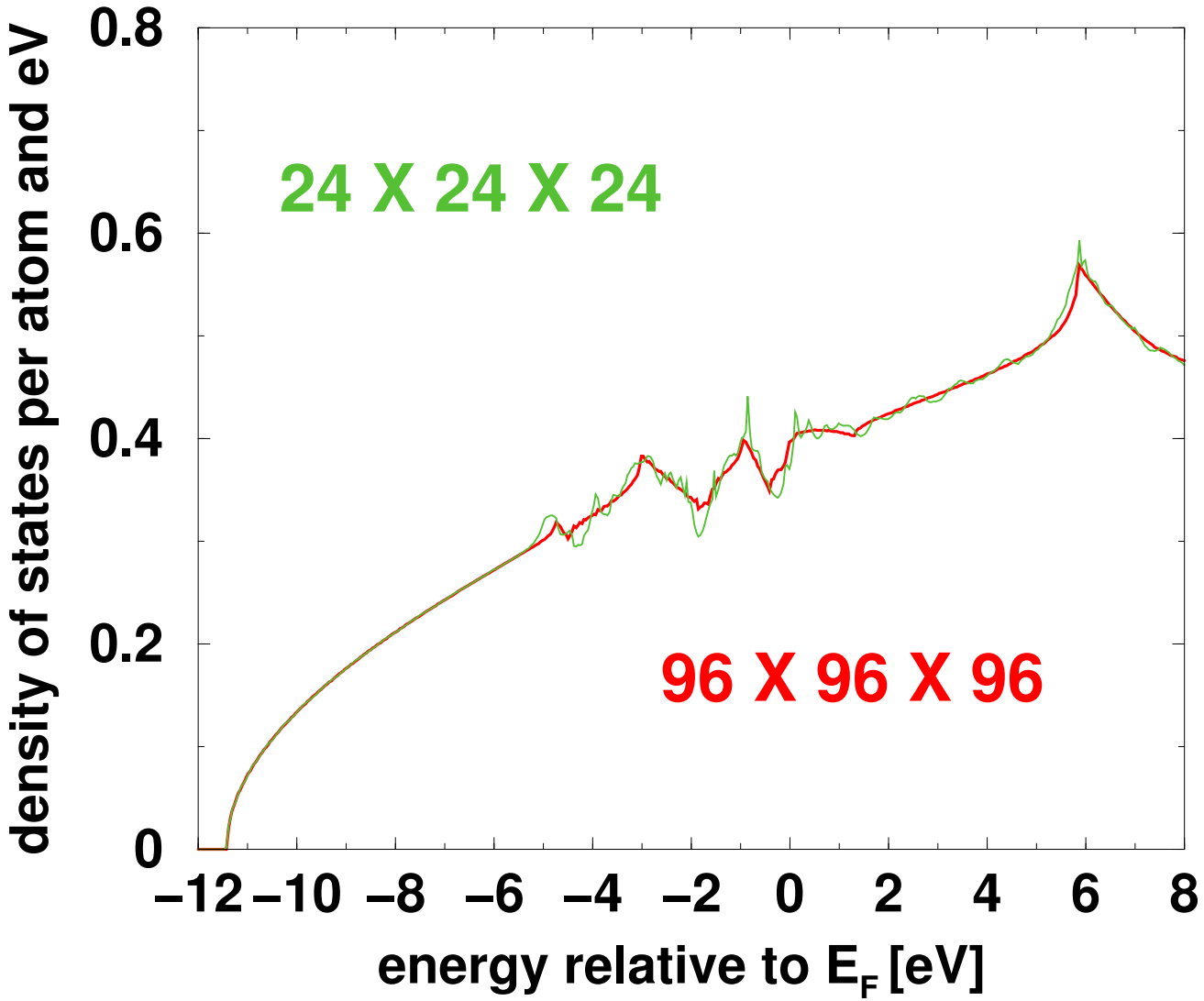
k-points in the full BZ	total energy [Hartree]
6 X 6 X 6	-241.92038912
12 X 12 X 12	-241.91919406
24 X 24 X 24	-241.91898968
48 X 48 X 48	-241.91902285
96 X 96 X 96	-241.91902497

Only the finest sampling ensures convergence at a level close to 10^{-6} Hartree.

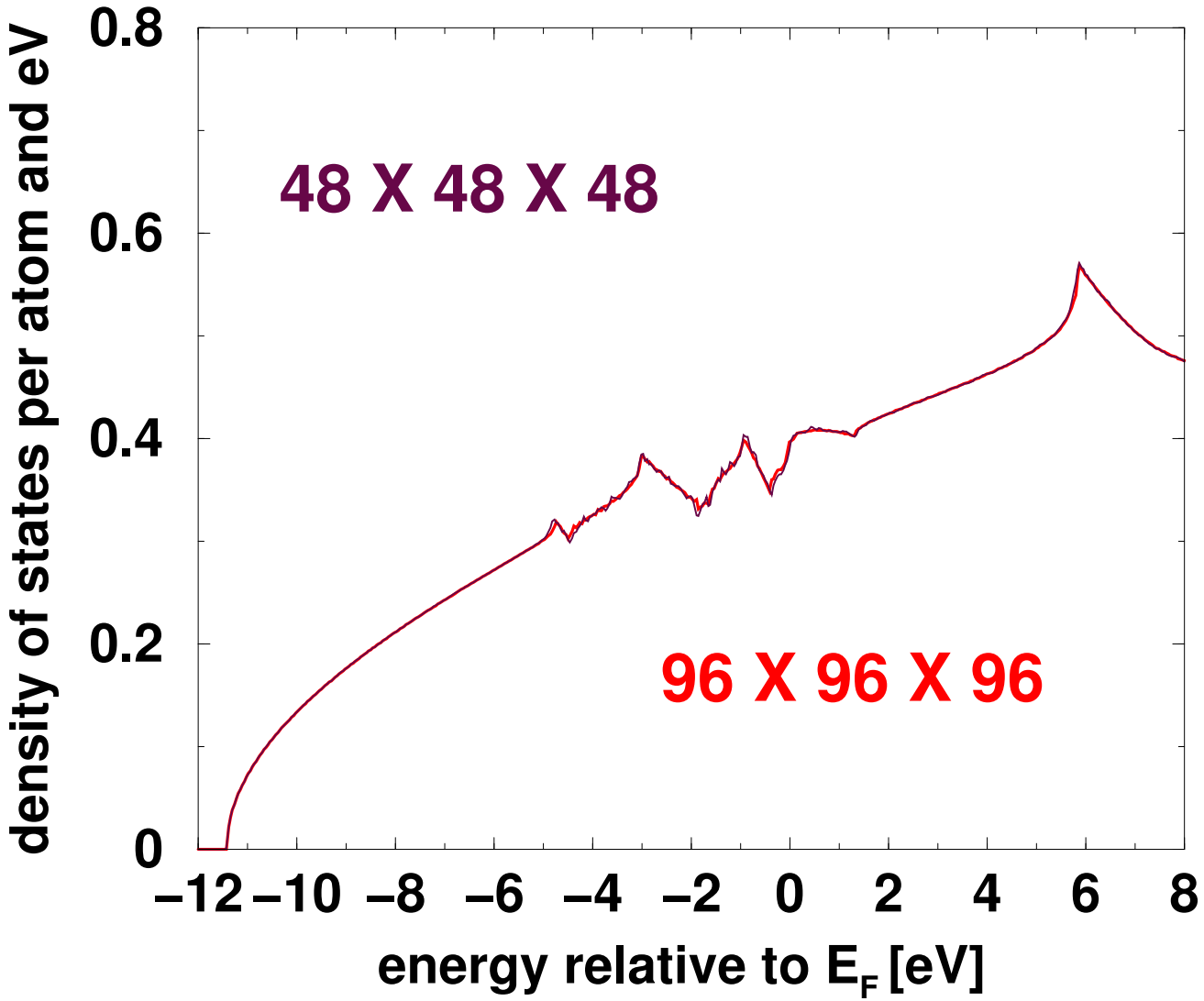
DOS of Aluminum with different k–point sampling



DOS of Aluminum with different k–point sampling



DOS of Aluminum with different k–point sampling



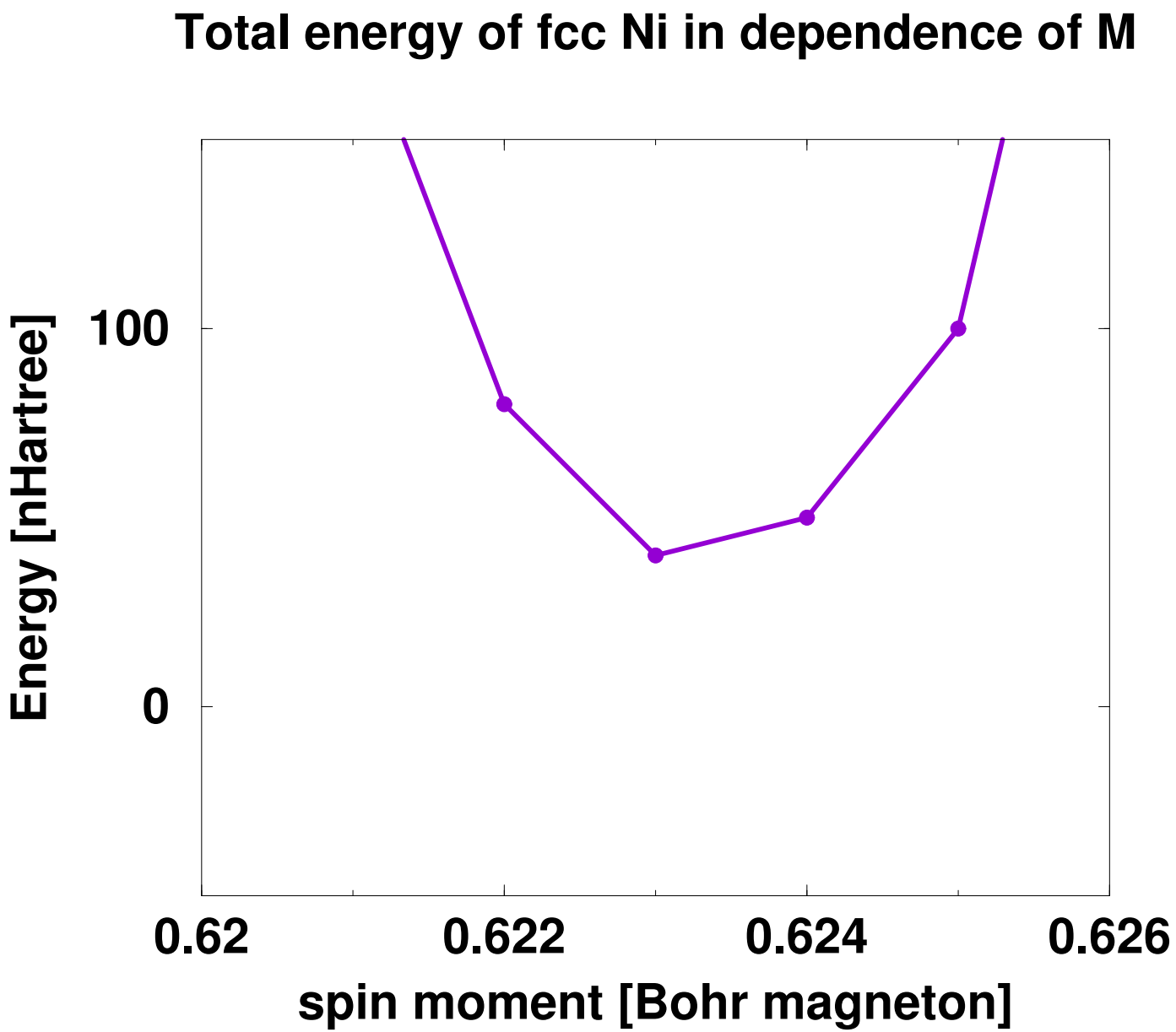
Nickel

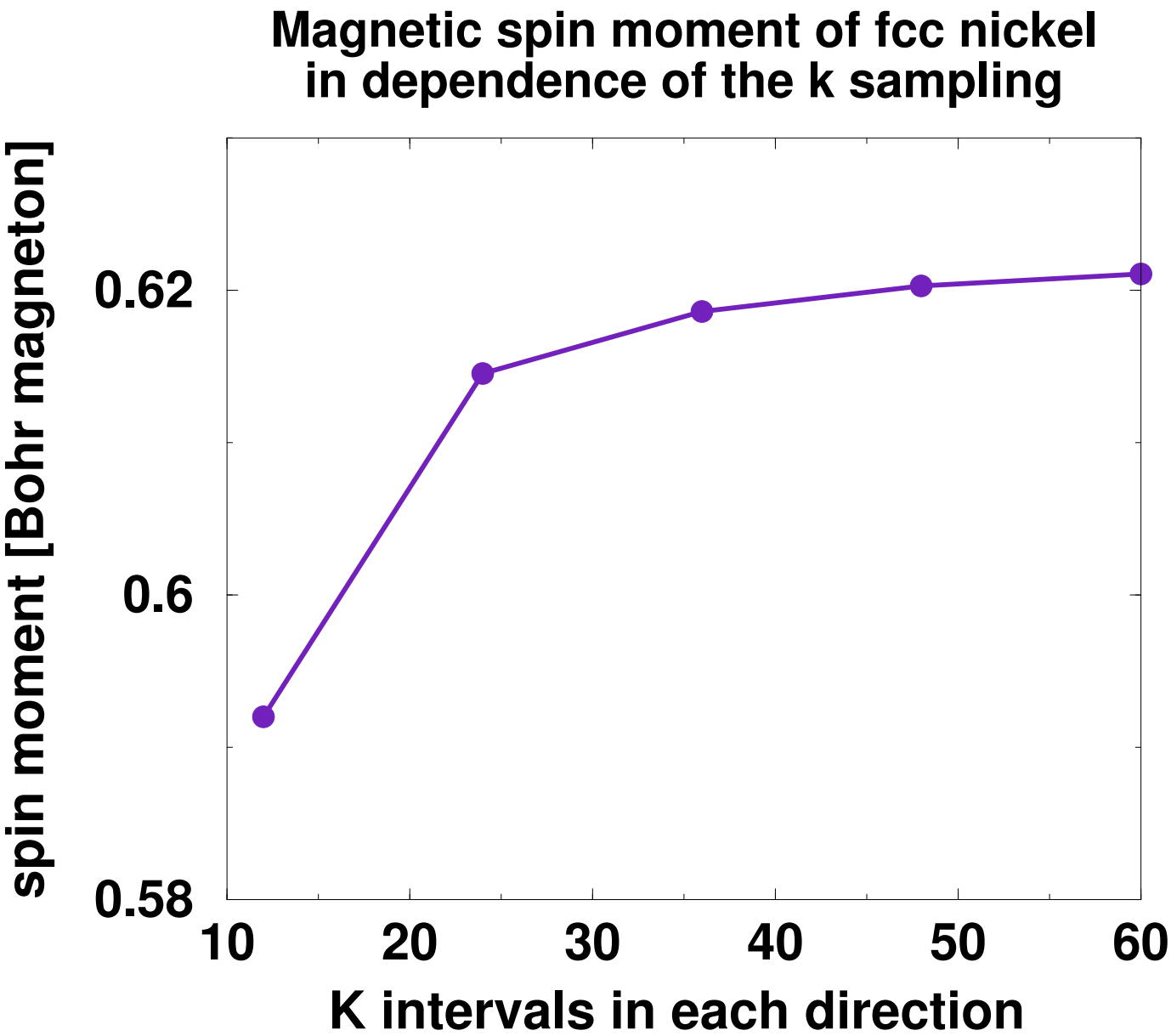
Fixed Spin Moment method:

spin moment constrained to a predefined value M. This allows to evaluate $E(M)$. Good for the determinatin of metastable magnetic states. In Nickel, only one (stable) ferromagnetic state exists.

FSM value of M_0 for 48 X 48 X 48 k-points: $0.623\mu_{\mathrm{B}}$

M_0 from an unconstrained calculation with the same sampling: $0.620\mu_{\mathrm{B}}$


Total energy of fcc Ni in dependence of M
Energy [nHartree]
100
0
0.62
0.622
0.624
0.626
spin moment [Bohr magneton]


Magnetic spin moment of fcc nickel
in dependence of the k sampling
spin moment [Bohr magneton]
0.62
0.6
0.58
10
20
30
40
50
60
K intervals in each direction