Task: Convergence of k-summation

Evaluate the total energy and the density of states of fcc aluminum versus the k-point number. Use a lattice constant of 7.53 **Bohr radii (close to the equilibrium lattice constant in LDA-PW 92). Use a strict convergence criterion (Density AND Energy). Use default settings else. Carry out four calculations with a subdivision of the Brillouin zone into 12 (default), 24, 48, and 96 intervalls in each direction.**

This task aims at providing a feeling for the dependence of total energy and details of the DOS on the **k**-point sampling. Hints:

(i) Create a new sub-directory for each calculation. Call the sub-directories k12, k24, k48, k96. Call the output files 'out'. You may speed up the calculation for the k=96 setting by using a converged charge density from one of the other calculations as input charge density:

[parent directory] cp k12/=.dens k96/=.dens

after convergence of the calculation running in k12.

(ii) You can check the convergence of the iterations by using the shell script 'grit':

[parent directory] grit k

yields a list of the distance between the final-iteration density vector and the previous density vector for all calculations running in the sub-directories k*.

(iii) You can extract the total energies (in Hartree) from the output files by using the shell script 'grEE':

[parent directory] grEE k

yields a list of the final-iteration total energies of k*/out. How many **k**-points do you need to get the total energy convered at a level of 10^{-6} Hartree?

(iv) If the calculations are converged, you can switch on the input option 'CALC_DOS' and re-run. Use:

[parent directory] xmgrace k12/+dos.total k96/+dos.total

to compare the densities of states for different **k**-point samplings. How many **k**-points do you need to get the DOS converged to about 10% accuracy?

Additional task on spin magnetism: How many **k**-points do you need to converge the spin moment of *fcc* Ni better than 0.01 μ_B?

Hints: space group 225; a = 3.5234 Å; switch "spin sorts" to "2" and activate the initial polarization in the main menu. If you use a pre-converged density (existing file =.dens), the initial polariztion has to be de-activated.

Solution: Convergence of k-summation (fplo8.65)

How many **k**-points do you need to get the total energy convered at a level of 10^{-6} Hartree?

k-points in the full BZ	total energy [Hartree]
$12 \times 12 \times 12$	-241.9194678655
$24 \times 24 \times 24$	-241.9192621143
$48 \times 48 \times 48$	-241.9192956648
$96 \times 96 \times 96$	-241.9192978375

Red color: digits that are not reliable due to restricted **k**-point sampling.

Only the finest sampling, $96 \times 96 \times 96$, ensures convergence at a level close to 10^{-6} Hartree.

How many **k**-points do you need to get the DOS converged to about 10% accuracy?
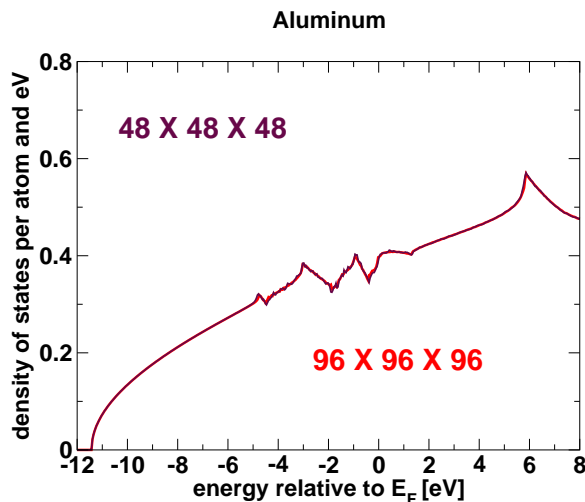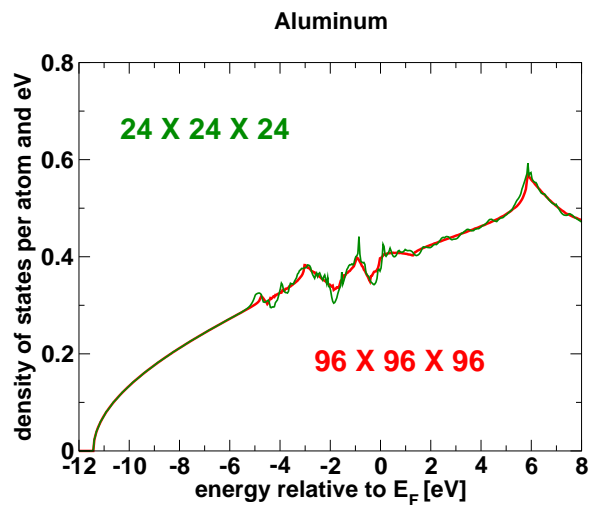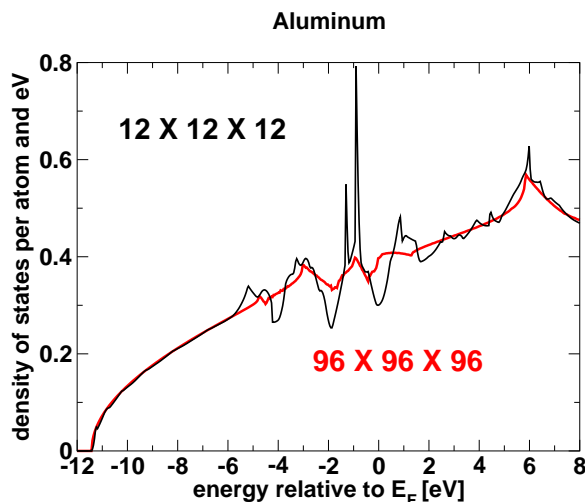
A DOS calculated with a sampling of $12 \times 12 \times 12$ ($24 \times 24 \times 24$, $48 \times 48 \times 48$) may deviate from a DOS calculated with a sampling of $96 \times 96 \times 96$ by 100% (10%, 1%).

How many **k**-points do you need to converge the spin moment of *fcc* Ni better than 0.01 μ_B?

k-points in the full BZ	total gross spin
$12 \times 12 \times 12$	0.5904
$24 \times 24 \times 24$	0.6129
$48 \times 48 \times 48$	0.6186
$96 \times 96 \times 96$	0.6202

Red color: digits that are not reliable due to restricted **k**-point sampling.

A sampling $48 \times 48 \times 48$ ensures convergence at a level of 0.01 μ_B (in the case of *fcc* nickel).