Lab1: Self-consistent calculation with QE

The goal of this lab is to learn the basic functionalities of a DFT method, i.e. running a selfconsistent energy cycle, calculates and plot densities of states and band structures. To this we use the Quantum Espresso code. During the onsite lab we will do together test calculations for one system. The homework will be based on this with small modifications, see below.

System

Our test system in LiMgN a Half-Heusler semiconductor which has been discussed for solar cell applications, see Fig. 1.



Figure 1: Building blockes of a Half-Heusler material. The half-Heusler structure is derived by combining rocksalt and zincblende structures. (Figure taken from Casper et al. Semicond. Sci. Technol. **27** (2012) 063001). In our case we have Mg on 4a, Li on 4b, and N on 4c sites.

Symmetry F43m (cubic), starting lattice constant a = 9.5 a.u..

The band gap of this materials can be tuned by replacing Mg or N with alternative elements. In your homework you will study one example replacing N by P.

Lab exercise (onsite):

1) Download the jupypter notebook Lab1-QE-SCF.ipynb from studium, put it in your docker and open it.

2) The first module is a simple selfconsistent cycle for fixed lattice constant and k-mesh.

- Before you start calculating, make sure you have the potentials which are used in the notebook. If not open the *AddingPseudoPotentials.nb* and add them.
- Carry out the cycle once.
- Take a look in the output file and search for the phrase:
 "highest occupied, lowest unoccupied level (ev):" These energy values define the band
- gap in eV.3) Now we know how a single cycle works, but we need to check the accuracy. Is the k-point density sufficient? To test this, we run over a loop with different k-point densities. The input
 - file is the same only k is a variable now.
 - Carry out the loop over several k-mesh densities. Use the plotting tool when finished. This should provide a E(k) plot which allows to decide which k-point mesh is sufficient for this case.
- 4) To calculate the band structure re-run the single selfconstent cycle with the appropriate k-point mesh obtained in 3).

- After this you run the non-selfconsistent calculation for the band structure. Use the Fermi energy ef according to your selfconsistent output.
- Plot the band structure.
- 5) To obtain the density of states we perform another non-selfconsistent run.
 - Make sure the input is correct (lattice constant, potentials etc .are the same as for the selfconsistent run).
 - Now we have to integrate over the full 1st BZ. To get a good DOS the k-point mesh must be denser as for the selfconsistent run. You can also change the smearing to get a smoother plot. Do your own testing.
 - Plot your DOS.

Homework:

Investigate the isoelectronic sister compound LiMgP.

- 1) Get a potential which fits to the other potentials. Check whether the cutoff is still ok. The values in the header of the potentials should be smaller than the ones in the input file.
- 2) Phosphorous is larger than N, so the lattice constant will change. To find the correct lattice constant, modify the k-mesh test cycle from our LiMgN example. You need to use the lattice constant (celldm) as variable instead of the k-point density. Do some rough testing with a few lattice constants and small k-mesh to find the approximate value. In the next step do an accurate calculation around this point for at least 5 different lattice constants.
- 3) Execute the EOS module attached to the notebook (end). You will get the volume and the bulk modulus.
- 4) Use the ground state lattice constant from 2) and perform a selfconsistent cycle. What is the band gap you get for LiMgP?
- 5) Do the band structure calculation for LiMgP. Plot it.
- 6) Calculate the DOS and plot it.

(In case you absolutely cannot manage 1) amd 2) use a= 6.025 Å as lattice constant and do the steps 3)-5).)