# CMS exercise 1: Wien2k

The primary goal of this exercise is to guide you through the main steps of a DFT calculation: the initial setup, a self-consistent calculation, and plotting density of states as well as the band structure. Calculations will be performed using the code wien2k version 14.2. As a step-by-step guide, please refer to the Chapter 3 of the wien2k documentation available at **www.wien2 k.at/reg_user/textbooks/usersguide.pdf**.

Upon completion of all tasks, please send the answers/plots to the numbered questions (in the margins) to J. Kunes (kunes@ifp.tuwien.ac.at).

To log in, please use the login name cms18_01, …, cms18_40 (mind the underscore symbol) and the password 41cms18. Please change the password (execute “passwd” in a terminal window) immediately after logging in. **Remember your login and new password**!

A few steps to configure wien2k for your account

1. Open a terminal window and execute /home/CMS/cms00/wien2k_14.2/userconfig_lapw”. Use the default settings.

2. Copy the bashrc_template to your home directory

cp /home/CMS/cms00/bashrc_template .bashrc

and **restart your session** (or open a new window)

3. open a new terminal window and run “w2web”. Choose a port number, e.g. the sum of the default port 7890 and your login number. Copy the URL and paste it into a browser window.

Important: to restart the server, open a terminal window, run “killall w2web” (don’t worry about the warnings) and then “w2web”.

# fcc Cu

Set up a calculation for fcc Cu

1. Create a new session called “Cu” and execute StructGen to create the structure file “Cu.struct”. Use the suggested parameters (RMTs, etc): lattice constant a=3.597 Å (fcc lattice)

2. Run the initialization. Use the GGA xc-potential (default option 13). Use between 500-1000 k-points.

3. Run an (spin) unpolarized self-consistent calculation. Use the charge density to control the convergence (<$10^{-6}$)

**Q1**: What is the Fermi energy? What is the total energy per Cu atom? How many atoms are in the primitive and in the conventional cells for fcc lattice?

4. Compute the band structure along the **Γ**-X-W-L-**Γ**-K cut through the Brilloouin zone. (use google to find what these letters mean, use Xcrysden to generate the k-path with 200-500 points).

**Q2**: Plot the band structure? Plot the 3d ‘fat’ bands (jtype=4 on line 11 or Cu.insp)? (Optional: Guess a formula to calculate the point size for the fat band plot)

5. Calculate the density of states (DOS). Create a denser k-mesh with *kgen* (10 000 k-points). Run the DOS calculation with *qtl* or *lapw2 -qtl*.

**Q3**: Plot the total density of states. What is the integral of DOS up to Fermi level (number and physical meaning)? Compute the projected DOS of 3d states. Check that it is consistent with the fat band plot.

6. Run Xcrysden (type xcrysden on the command line) to visualize the Fermi surface: Open Wien2k -> Fermi Surface and follow the instructions.

**Q4:** Plot the Fermi surface (note that you have to select the sheet/band to plot - here it is simple because there is only a single sheet). What is the geometric meaning of the Fermi surface?

# bcc Fe (spin polarized)

Set up a calculation for bcc Fe

1. Create a new session called “Fe” and execute StructGen to create the structure file “Fe.struct”. Use the suggested parameters (RMTs, etc). lattice constant a=2.856 Å (bcc lattice)
2. Run the initialization. Use the GGA xc-potential (default option 13). Use between 500-1000 k-points.

3. Run an (spin) uppolarized self-consistent calculation. Use the total energy to control the convergence ($<10^{-4}$)

4. Set up another session with the same parameters. Run a spin polarized calculation.

**Q5:** What are the total energies for the polarized and unpolarized calculations? What conclusion can one draw from them? What is the ordered spin moment per Fe atom?

# Optional

Experiment with the computational parameters: e.g. plot the DOS for different k-meshes, investigate the dependence of total energy on RMT and basis size RMT*KMAX

Calculate the E(V) energy vs volume curve for fcc Cu, i.e. perform calculations for several different lattice constants. Make sure that the RMT is small enough to accommodate the most compressed structure.

# NiO

Set up a calculation for NiO

rock-salt structure: fcc lattice  Ni (0,0,0), O(1/2,0,0)

use standard settings, run unpolarized calculation