Exercise 1: Getting started:

- Account information (username/pw): kursXX / wien2k
  - *(for XX put the numbers shown on your pc)*
- ----------
- i) Open a terminal window.
- ii) Start w2web (accept all defaults, specify kursXX / wien2k for account)
- iii) Connect with firefox to w2web as indicated on the screen of ii)
- iv) Try the "quick-start" example for TiC as described in the UG
  - *structgen*
  - *init_lapw*
  - *scf-cycle (run_lapw)*
  - *analyse (:ENE, :DIS, :CTO) graphically*
  - *save_lapw*
  - *electron density (valence density without Ti-semicore; difference density)*
  - *DOS (Ti eg,t2g, C s,p)*
  - *bandstructure (with "character plotting")*

Exercises 2: Testing accuracy: RKmax and k-points

- Use the TiC example and calculate the equilibrium volume ("optimize") using:
  - *RKmax=5 100 k-points / RKmax=7 100 k-points / RKmax=7 1000 k-points*
- a) run x optimize and generate 5 structures (-6, -3, 0, 3, 6 % volume change)
- b) set RKMAX=5 in TiC.in1 and x kgen with 100 k-points
- c) edit "optimize.job". Modify the "save_lapw" command to:
  - *save_lapw ${i}_rk5_100k*
- d) run optimize.job, plot the results
- e) set RKMAX=7 in TiC.in1
- f) edit "optimize.job". Uncomment the cp line and modify:
  - *cp ${i}_rk5_100k.clmsum TiC.clmsum # This saves lot of CPU time!!*
  - *...*
  - *save_lapw ${i}_rk7_100k*
- g) repeat step d) (plot the results for "*_rk7_100k")
- h) x kgen (with 1000 k-points)
- i) repeat steps f) and g) with proper modifications

- Remember: Depending on the specific property you want to calculate (just a DOS, or Energy-Volume curves, or EFG, or structure optimization with forces,..) and the desired accuracy, the types of atoms, insulator/metal and system size you may need:
  - *H: RKmax > 2.5; sp-elements: RKmax > 5; d-elements: RKmax > 6; f-elements: RKmax > 7;*
  - *1 atom/cell, metal: 1000-10000 k-points or more*
  - *1 atom/cell, insulator: 100-1000 k-points or more*
  - *For N atoms/cell you can reduce the k-mesh by a factor N*

- Remember: Always test your **specific property** for convergence !!

Exercise 3:

- optimization of positions: rutile TiO_2:
  - *P42/mnm (136), a=4.59 c=2.96 Å; Ti(0,0,0) O(0.3,0.3,0)*
  - *init_lapw: (setrmt -2%; 100k, RKmax=6.5)*
  - *min_lapw (use NEW1 and 1.0 in case.inM)*
    - analyze :ENE :FGL002 :POS002 :EFG001 in case.scf_mini (exp. pos:0.305)
- Supercells:
  - *Create a small supercell (eg. TiC P-lattice; TiO_2 1x1x2; simple surface) using "x supercell" and "modify" the supercell (vacancy, impurity)*
- X-ray emission/absorption spectroscopy
  - *use final TiO2 structure, finer k-mesh,*
  - *XSPEC task for O-K and Ti-L2 spectra*
- Relativistic effects (SO) + optics: fcc Au, a_0=4.08 Å
  - *scalar-relativistic calculation; save_lapw, fine k-mesh (5000-50000k); DOS + optics*
  - *reset k-mesh; initso; run_lapw –so; save_lapw; fine k-mesh, DOS + optics -so*

Exercise 4:

- Magnetism: bcc Fe (a_0=2.86 Å)
  - *5000k; spin-polarization:yes*
  - *do a volume optimization (-6, -3, 0, 3, 6 %)*
    - check equillibrium volume, :MMT as function of volume
    - compare bandstructure and DOS for large/small volumes (use restore_lapw; x lapw0)
- Antiferromagnetism: bcc Cr (a_0=2.885 Å)
  - *compare a ferromagnetic (bcc cell with 1 Cr) with*
  - *antiferromagnetic calculation (P cell with Cr1 and Cr2 (at 0.5,0.5,0.5))*
    - for afminput your symmetry operation is "identity+(0.5,0.5,0.5)"
- LDA+U: NiO: NaCl structure, A-type AFM along 111 →
  - R-cell: 5.605236 5.605236 27.459934 bohr
  - Ni1 (0,0,0), Ni2 (0.5,0.5,0.5), O ±(.25,.25,.25) (flip spin for Ni2) (view the structure in Xcrysden !)
  - GGA and GGA+U calculations, (use U=6eV, J=0; check the UG to understand case.inorb/indm)
  - compare DOS for GGA and GGA+U