

# Exercise 1: Getting started:



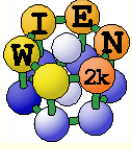
- Account information (username/pw): kursXX / wien2k
  - *(for XX put the numbers shown on your pc)*
- -----
- i) Open a terminal window.
- ii) Start w2web (accept all defaults, specify kursXX / wien2k for account)
- iii) Connect with firefox to w2web as indicated on the screen of ii)
- iv) Try the "quick-start" 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  $\text{TiO}_2$ :**
  - $P42/mnm$  (136),  $a=4.59$   $c=2.96$  Å;  $\text{Ti}(0,0,0)$   $\text{O}(0.3,0.3,0)$
  - *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.  $\text{TiC}$  P-lattice;  $\text{TiO}_2$  1x1x2; simple surface) using "x supercell" and "modify" the supercell (vacancy, impurity)
- **X-ray emission/absorption spectroscopy**
  - use final  $\text{TiO}_2$  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 ( $a_0=2.86 \text{ \AA}$ )**
  - *5000k; spin-polarization:yes*
  - *do a volume optimization (-6, -3, 0, 3, 6 %)*
    - check equilibrium volume, :MMT as function of volume
    - compare bandstructure and DOS for large/small volumes (use restore\_lapw; x lapw0)
- **Antiferromagnetism: bcc Cr ( $a_0=2.885 \text{ \AA}$ )**
  - *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  $\pm(.25,.25,.25)$  (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