connect/setup of w2web environment

- Connect to **pleiades.bc.edu** using **NoMachine** as indicated in the instructions and with the username/pw you got during registration.

- open a terminal and connect to your compute node using:
  - *ssh -Y compute-4-X (X was given during registration)*

- start w2web on port 66yy and a firefox browser using:
  - *runwien2k.pl 66yy (where yy corresponds to your wienyy username)*
    - the first time you have to enter user-id/pw (use the same as for your login) and also the port 66yy.
    - firefox connects automatically to http:compute-4-X:66yy
    - note that when you kill firefox, also the w2web server will be stopped.

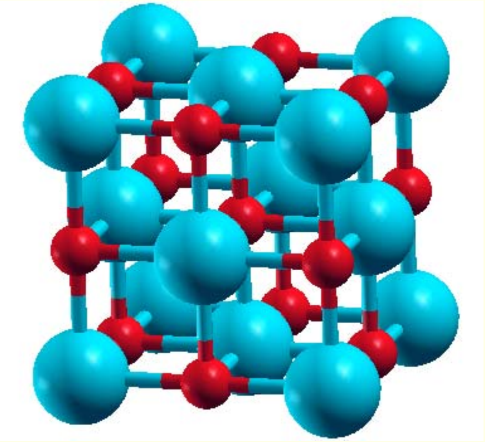
- Start with the exercises.

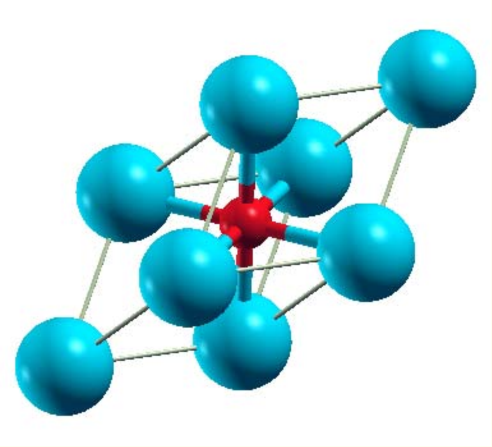
Exercises:

- In the following you find some suggestions for exercises, which teach you various tasks one may perform with WIEN2k.
- New WIEN2k users should start with the first basic exercises (1-5), covering: structure generation, initialization, scf-cycle, bandstructure, DOS, electron density, structure optimization, supercell generation, spin polarization
- Later on, choose examples of your interest as there are probably more exercises than you can do here.
- Please note, that often "calculational parameters" are set to "minimal cpu-time" instead of "fully converged calculations".
- Do not use such small values for final results and publications without convergence checks !!

Exercise 1: Getting started:

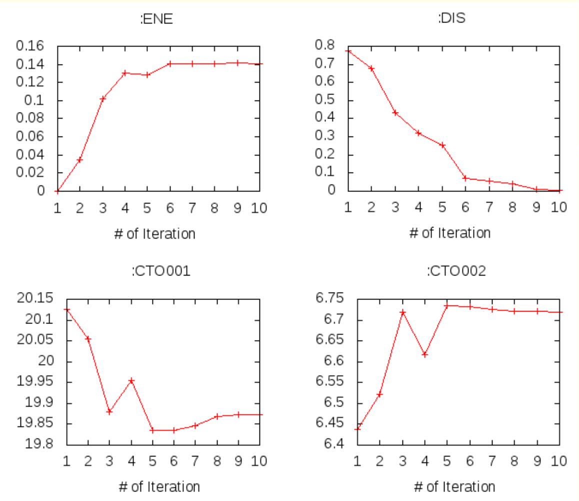
- i) Open a terminal window (skip points i-iii if done before)
- ii) Start w2web (accept all defaults, specify account, port)
- iii) Connect with firefox to w2web as indicated on the screen of ii)
- iv) Try the "quick-start" example for **TiN** (similar to TiC in the UG)
  - *create new session named "TiN", "create" and "select" the suggested directory.*
  - *Generate structure (a=4.235 Ang; reduce RMT by 1%)*
  - *view structure with Xcrysden (switch primitive / conventional cell)*



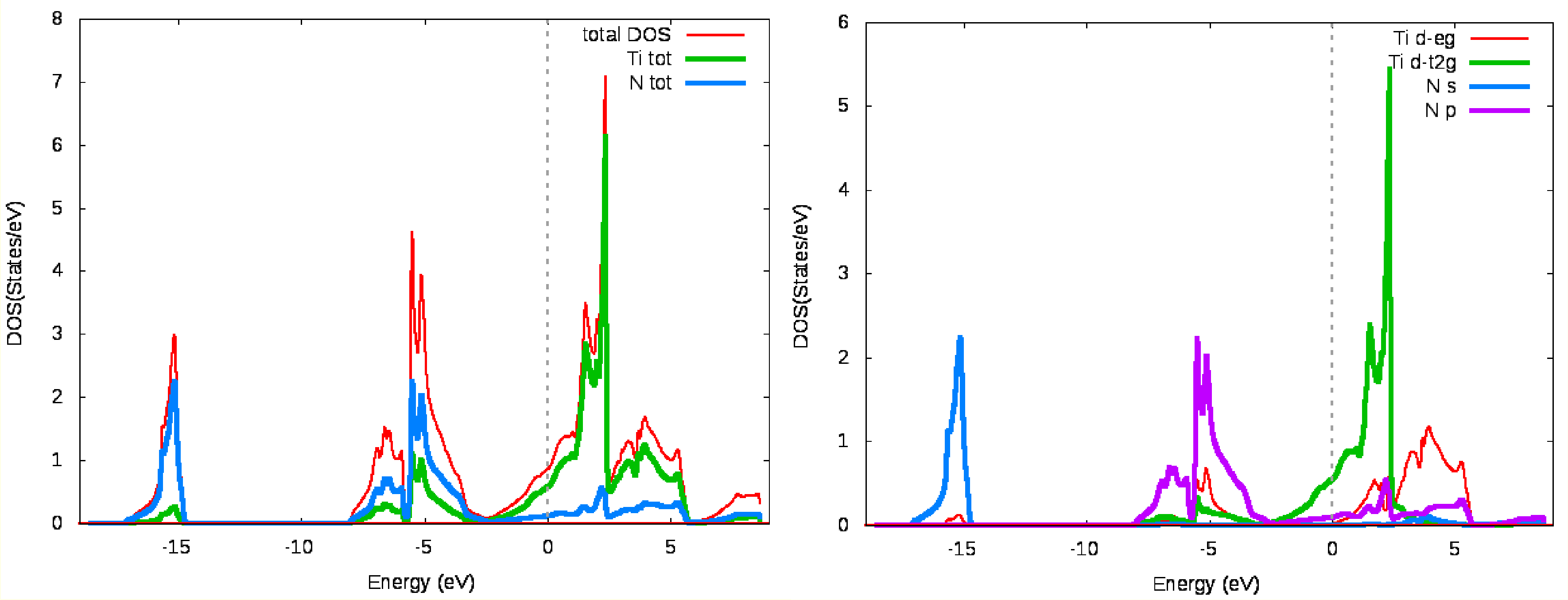


  - *initialize (init_lapw -b); use defaults*
  - *scf-cycle (run_lapw); use defaults; monitor "STDOUT" and "dayfile"*
    - How many iterations did you need ? How long took a single scf-iteration ?

TiN continued



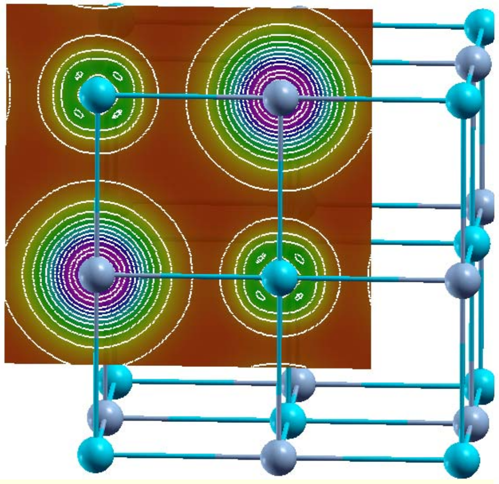
- *utilities: analyse*
  - (:ENE, :DIS, :CTO) graphically
- *utilities: save_lapw (use as save-name: "TiN_exp_pbe_rk7_1000k")*
- *DOS (plot 7 cases: total + Ti-tot + N-tot and Ti-eg + Ti-t2g + N-s + N-p)*



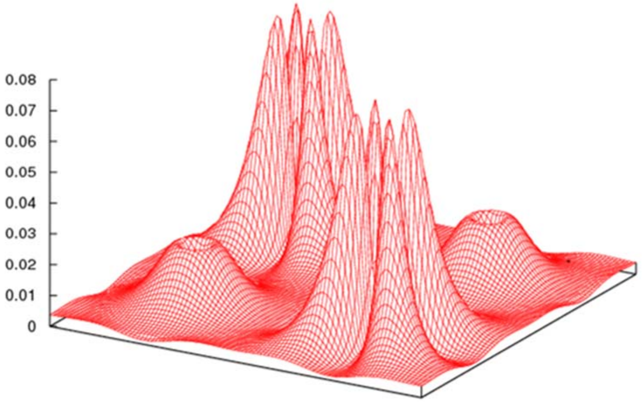
TiN continued …

- *electron density (use xcrysden to select the (100) plane), view it in xcrysden and rhoplot to "understand contour and 3D-plots")*
  - **valence** density (without semicore, check TiN.scf1 to find a EMIN which truncates the Ti-3s,3p states); compare the density around Ti with TiC (UG)
  - **difference** density (observe "charge transfer" and "t_{2g}-anisotropy" around Ti)
  - densities of the "**N-p**" and "**occupied Ti-d-band**" (get the corresponding E-intervals from DOS-plots (in Ry!) and use these energies in the "x lapw2" step; observe the e_g and t_{2g} asymmetry around Ti and the different N-p "weights", explain the chemical bonding

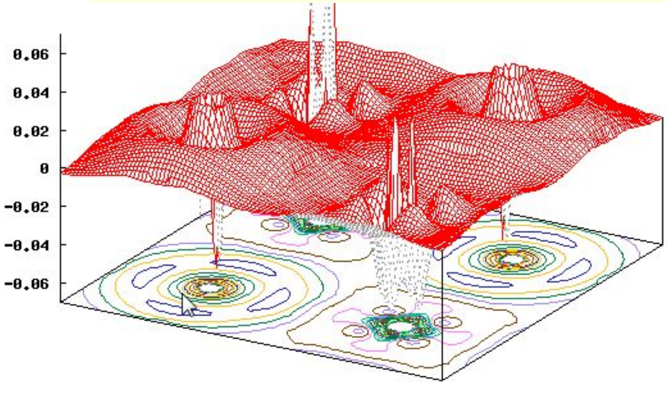
valence ρ



Ti-d band

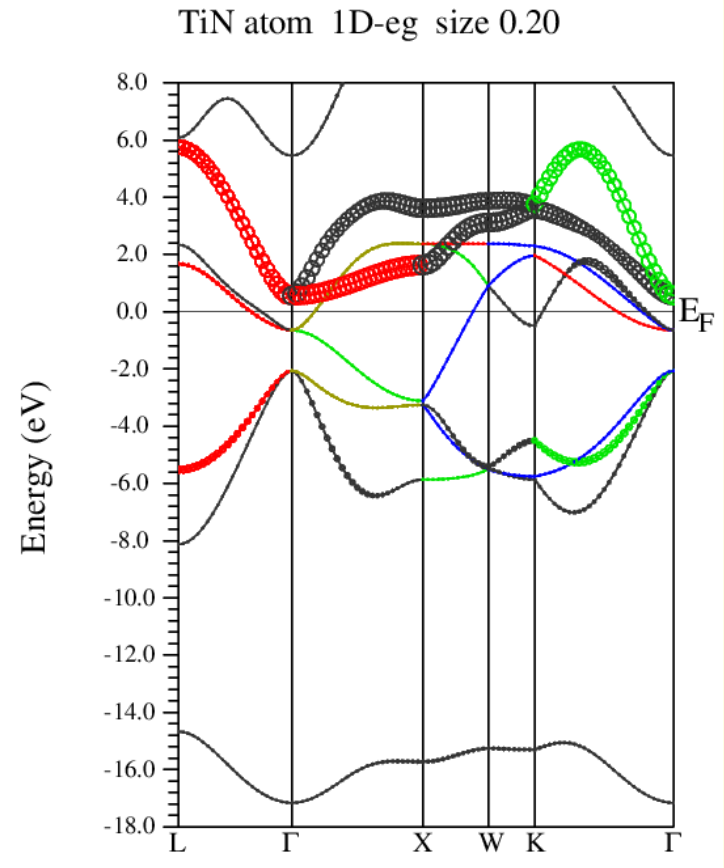


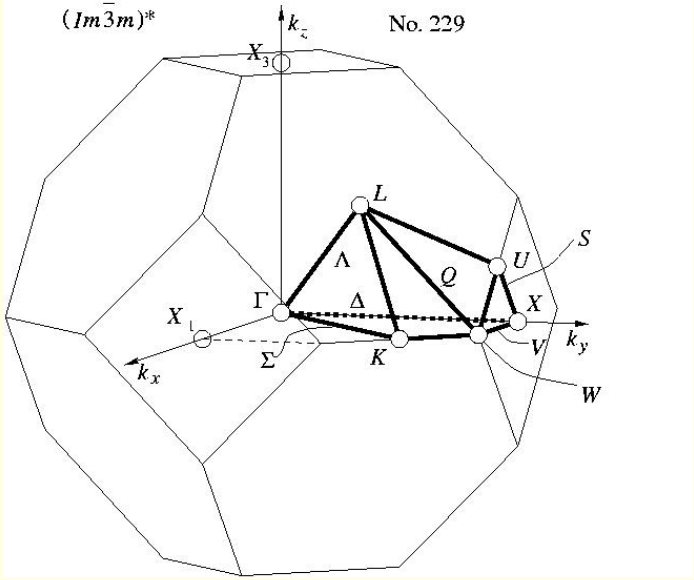
difference density



TiN continued

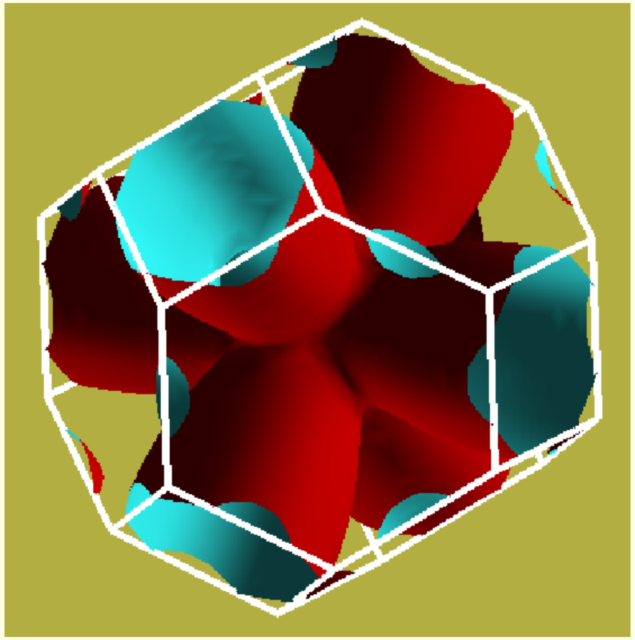
- bandstructure (along L-Gamma-X-W-K-Gamma with “character plotting”)
  - *use xcrysden (save as „xcrysden.klist“; select „from xcrysden“ in next step and click generate k-mesh)*
  - *identify “t2g-” and “eg-” bands (fat band plots)*





TiN continued …

- *Fermi surfaces*
  - open a terminal, change into the TiN directory and issue:
  - `xcrysden --wien_fermisurface .`
    - choose a good k-mesh (eg. 10000 points);
    - plot the FS for all bands (**9**, 10,11) which cross E_F and compare to band structure



Exercises 2: lattice parameter of TiC
Testing accuracy: RKmax and k-points

- TiC (fcc, **a=4.328** Ang, **setrmt 4%**)
- a) initialize in expert mode with **LDA, RKmax=5, 200 k-points** (bad values !!)
- b) run x optimize and generate 6 structures (-12, -9, -6, -3, 0, 3% change)
  - *(because of LDA we expect 1-2% smaller lattice parameter (3-8% in volume) than experiment)*
- c) edit "optimize.job". Modify “run_lapw” and "save_lapw" commands to:
  - *run_lapw –cc 0.001 –ec 0.00001*
  - *save_lapw ${i}_default_rkm5_200k*
- d) run optimize.job, plot the results (using *rkm5_200k)

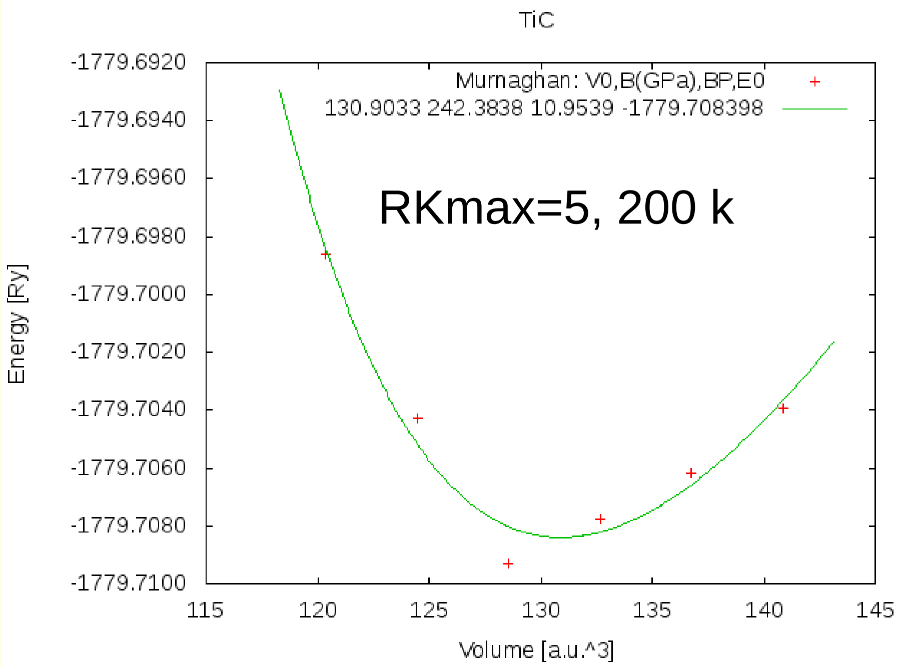
- e) set **RKMAX=6.5** in TiC.in1 and x kgen with **1000k**
- f) edit "optimize.job“: **Uncomment** the “**cp line”** and **“comment clmextrapol”**, change the save statement:
  - *cp ${i}_default_rkm5_200k.clmsum TiC.clmsum # Using previously converged densities saves a lot of CPU time!!*
  - *# clmextrapol ...*
  - *save_lapw ${i}_default_rkm6.5_1000k*
- g) repeat step d) (plot the results for “*_rkm6.5_1000k”)

Volume optimization for TiC

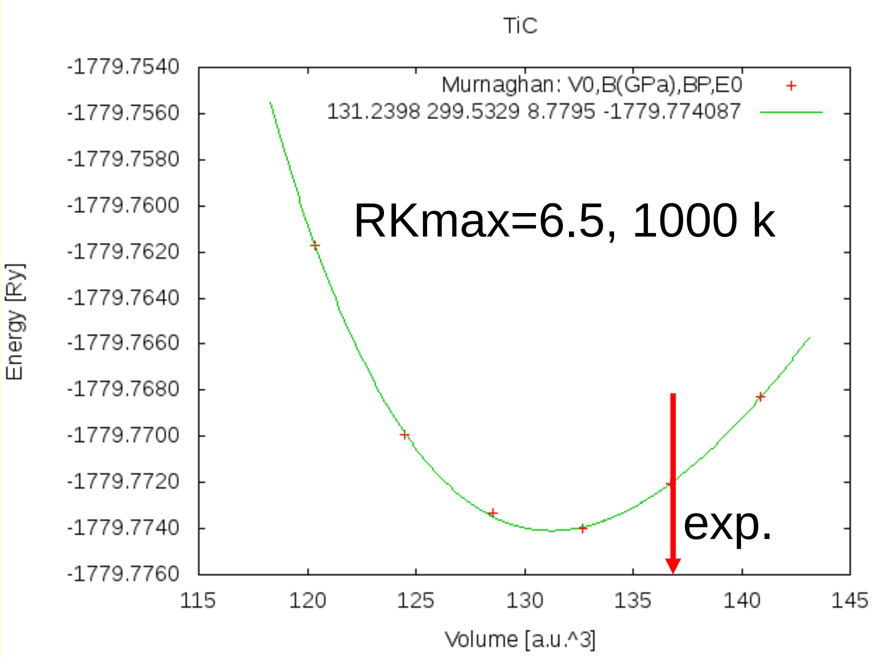
- (Non)-converged RKmax and k-points lead to smooth/non-smooth curves.
- Fully converged results require Rkmax ~ 9 , 10000 k and 10 volumes with ∆V=1%.
- Another XC-potential (eg. PBEsol) will drastically change a_0.

Remember: Always test convergence for your **specific property** !!
Different properties may require different parameters.
Different types of atoms, insulator/metal and system size may need different parameters:

H: RKmax > 2.5; sp-elements: RKmax > 5; d-elements: RKmax > 6; f-elements: RKmax > 7; (see our faq-page)
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



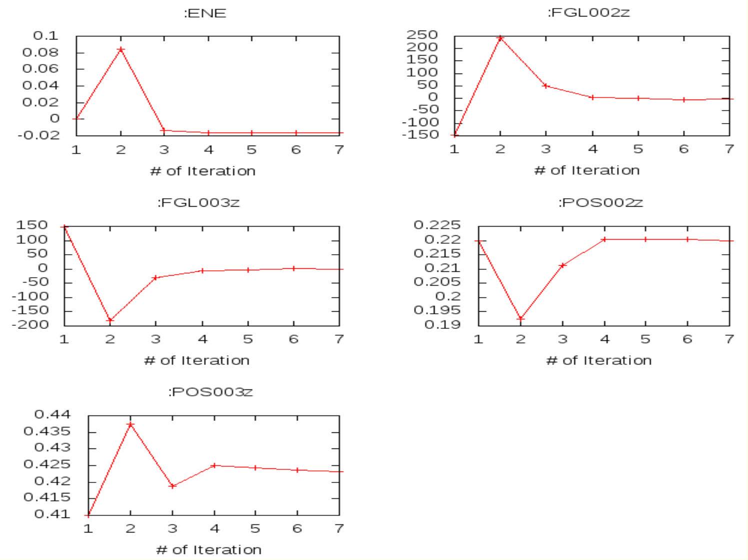
RKmax=5, 200 k

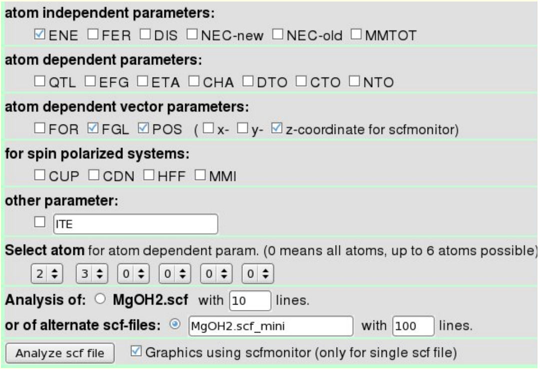


RKmax=6.5, 1000 k

Exercise 3: optimization of positions in Mg(OH)$_2$

- **create two “cases” (directories) for PORT and MSR1a optimization**
  - *initialize both cases (or copy after init one case to the other and use „rename_files")*
  - *P-3m1 (164), a=b=3.15 c=4.77 Å γ=120º; Mg(0,0,0)   O(1/3,2/3,**0.22**) H(1/3,2/3,**0.41**);   RMT: reduce by 7%*
  - *init_lapw -b –numk 100 –rkmax 3*
- **minimization using PORT:**
  - *min_lapw (or „mini-positions in w2web)*
  - *save_lapw case_relaxed_rkm3*
  - *analyze **case.scf_mini***
    - :ENE :FGL002z :POS002z :FGL003z :POS003z
  - *Find out how many scf cycles you needed*
    - grepline :ITE '*scf‘ 1   (in terminal)
- **check RKMAX convergence:**
  - *increase RKMAX to 3.5 (case.in1)*
  - *run –fc 1   (and check your forces)*




atom independent parameters:

☑ ENE ☐ FER ☐ DIS ☐ NEC-new ☐ NEC-old ☐ MMTOT

atom dependent parameters:

☐ QTL ☐ EFG ☐ ETA ☐ CHA ☐ DTO ☐ CTO ☐ NTO

atom dependent vector parameters:

☐ FOR ☑ FGL ☑ POS (☐ x- ☐ y- ☑ z-coordinate for scfmonitor)

for spin polarized systems:

☐ CUP ☐ CDN ☐ HFF ☐ MMI

other parameter:

☐ ITE

Select atom for atom dependent param. (0 means all atoms, up to 6 atoms possible)

2 3 0 0 0 0

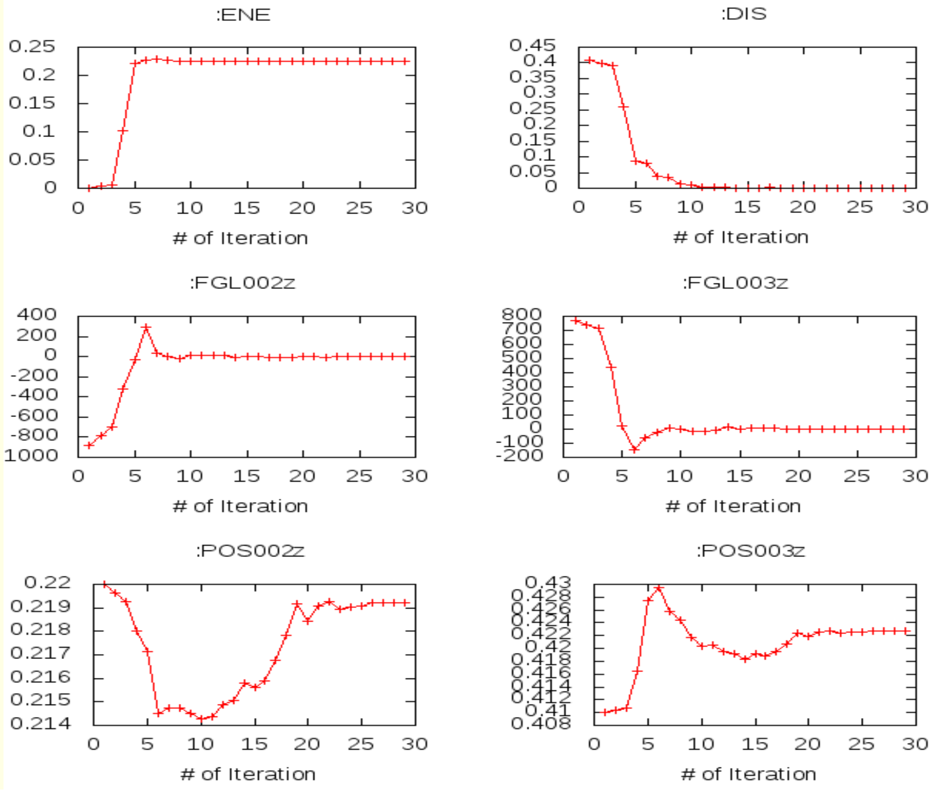
Analysis of: ○ **MgOH2.scf** with 10 lines.

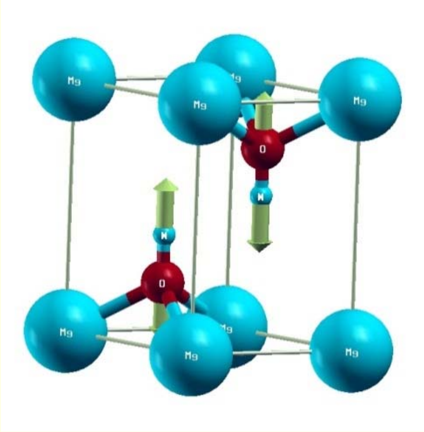
or of alternate scf-files: ● MgOH2.scf_mini with 100 lines.

☑ Graphics using scfmonitor (only for single scf file)

Mg(OH)$_2$ continue

- minimization using MSR1a:
  - ***run -min –fc 1 –cc 0.001 –ec 0.0001***
    - -min sets MSR1a in case.inm, (sometimes a crude scf cycle to come closer to „Born-Oppenheimer" surface is necessary (run -fc 20)
  - *analyze* ***case.scf*** and find out how many scf cycles you needed
    - :ENE :FGL002z :POS002z :FGL003z :POS003z :ITE
  - *save_lapw case_final*
  - *use the „arrows" utility to display initial forces and final relaxations (see UG p.195)*





Exercise 4: Creation of supercells

- These exercises should be done WITHOUT w2web in a terminal window !
- **creation of basic structure: MgO**
- mkdir super; cd super;
- makestruct (and type in the following information). It creates **init.struct**
  - *MgO: lattice type: F, a= 7.96 bohr*
  - *Mg (0,0,0), O (0.5,0.5, 0.5)*
- cp init.struct super.struct
- view the structure using: xcrysden --wien_struct init.struct

- **16-atom supercell**
- x supercell (use **super.struct**, select **2x2x2** and **F-cell):**
- cp super_super.struct super.struct
- edit super.struct and mark first Mg atom as "**Mg1**"
- x nn and if :WARNINGs appear do the next line:
  - *cp super.struct_nn super.struct; and repeat the "x nn" step above*
- x sgroup and view super.outputsgroup (no errors, but gives you a spacegroup)
  - *how many non-equivalent atoms do you have now ? view the structure with xcrysden. Now you would be ready to run **init_lapw -b ....,** but we just save it using **cp super.struct super_16.struct***

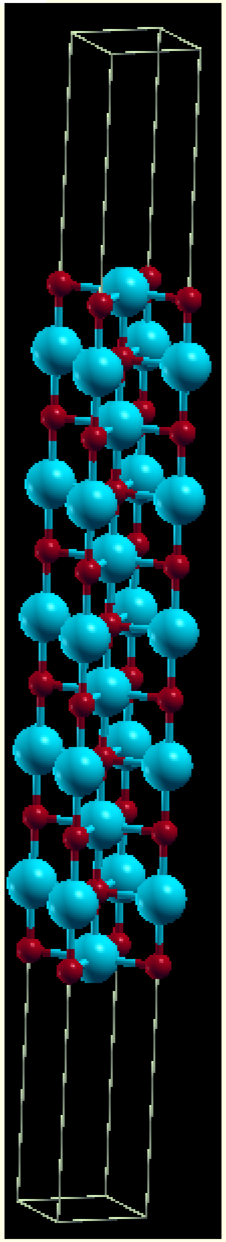
Exercise 4: Creation of supercells (cont.)

- **32, 64 and 128-atom supercells** (as above, but with B, P cell or 4x4x4-F)
- cp init.struct super.struct
- x supercell (use **super.struct**, …**):**
- cp super_super.struct super.struct
- edit super.struct and mark first Mg atom as "**Mg1**"
- x nn and if :WARNINGs appear do the next line:
  - *cp super.struct_nn super.struct; and repeat the "x nn" step above*
- x sgroup and view super.outputsgroup (no errors, but gives you a spacegroup)
  - *how many non-equivalent atoms do you have now ? view the structure with xcrysden. Now you would be ready to run i**nit_lapw -b ...., (see eg. lecture on XANES spectroscopy)***
  - *save the structures using **cp super.struct super_32.struct***

- Instead of labelling "Mg1", one could also **remove** an atom (vacancy) or **replace** an atom by another (impurity).
- Replacing atoms is better done in w2web, because this will also update radial meshes. (change **name** of atom AND **remove Z** !!)

Exercise 4: Creation of surface slabs, relax it

- **(001) surface with 11 layers:**
- mkdir 001, cp init.struct 001/001.struct; cd 001
- x supercell (use **001.struct**, 1x1x5, 30 bohr vacuum in z; repeat atom at 0:y)**:**
- cp 001_super.struct 001.struct
- xcrysden --wien_struct 001_super.struct & (leave it open for comparison)
- x sgroup and view 001.outputsgroup (it created a new structure for you)
- cp 001.struct_sgroup 001.struct
- xcrysden --wien_struct 001.struct
  - *what has sgroup done ?? how many total and non-equivalent atoms and how many **atoms/layer** do you have before/after sgroup ? Do you have inversion symmetry ?*
  - *save the structure using **cp 001.struct start_surface-001.struct***
- init_lapw –b –numk 10 –fermit 0.002 # 2D-BZ !
- run_lapw –fc 10 # observe the forces in scf-file, what relaxation do you expect ?
- save_lapw unrelaxed
- run_lapw –min –fc 1 # minimizes forces by optimizing positions
- save_lapw relaxed
  - *How much have the surface and sub-surface atoms relaxed ?*



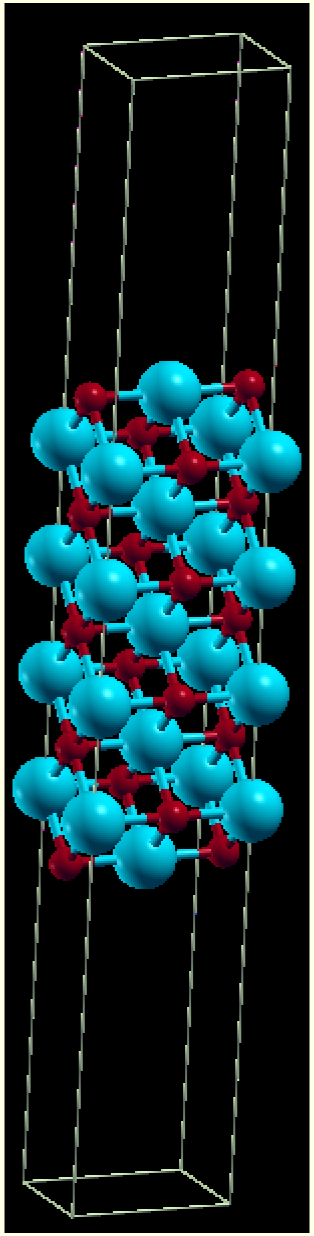
add-atoms, bigger cells, …

- If you now want to study **adsorption** of an atom you could simply add **2 equivalent** atoms manually (this is much easier in w2web, since the struct file is position dependent !!) at a suitable starting position, eg. (0,0,+/-z) (2 atoms to keep inversion symmetry !!)
  - *where would you add two Fe atoms ?*
  - *at what distance ?*
  - *check it out using xcrysden*

- This structure could then serve as base for a bigger supercell (for instance 2x2x1) to simulate reduced “coverage”.

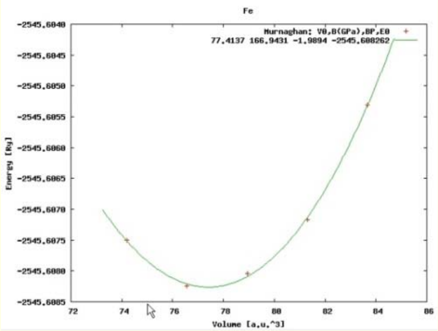
Exercise 4: Creation of supercells (cont.)

- **(110) surface with 9 layers: (**using the **structeditor)**
- octave (use repeat-key arrow-up !)
  - *helpstruct* *# list all possible commands*
  - *a=loadstruct("init.struct");*
  - *ac=makeconventional(a);* *# convert F into P cell*
  - *help makesurface* *# explains the syntax*
  - *sr=makesurface(ac, [1 1 0], 1, 20., 30.);*
  - *showstruct(sr)* *# check out the number of layers and repeat the **sr=makesurface** command with larger thickness until you get 9 layers. How do you get an O-atom at the origin ?*
  - *savestruct(sr,"super.struct")*
  - *quit*
- xcrysden --wien_struct super.struct &
- x sgroup and view super.outputsgroup
- cp super.struct_sgroup super.struct
- xcrysden --wien_struct super.struct
  - *what has sgroup done ?? how many total and non-equivalent atoms and how many **atoms/layer** do you have before/after sgroup ? Do you have inversion symmetry ?*
  - *save the structure using **cp super.struct super_surface-110.struct***



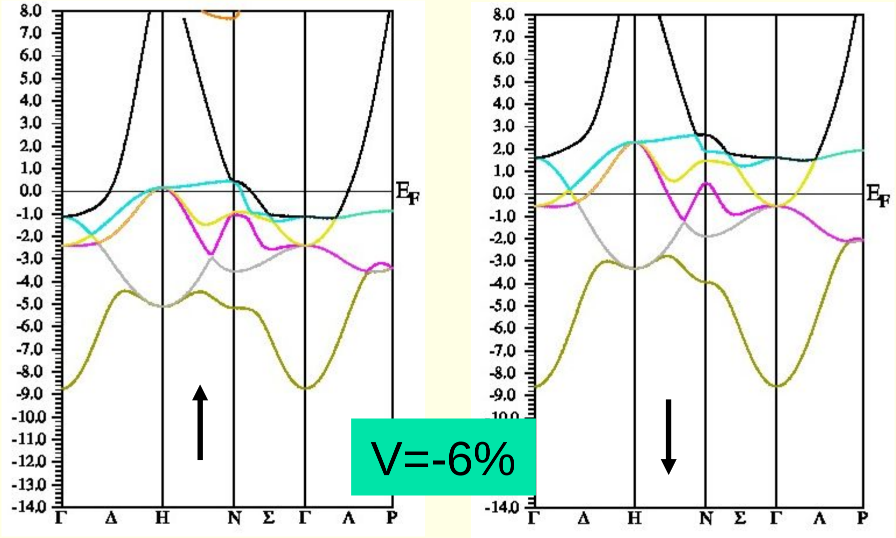
Exercise 5: spin-polarized calculations

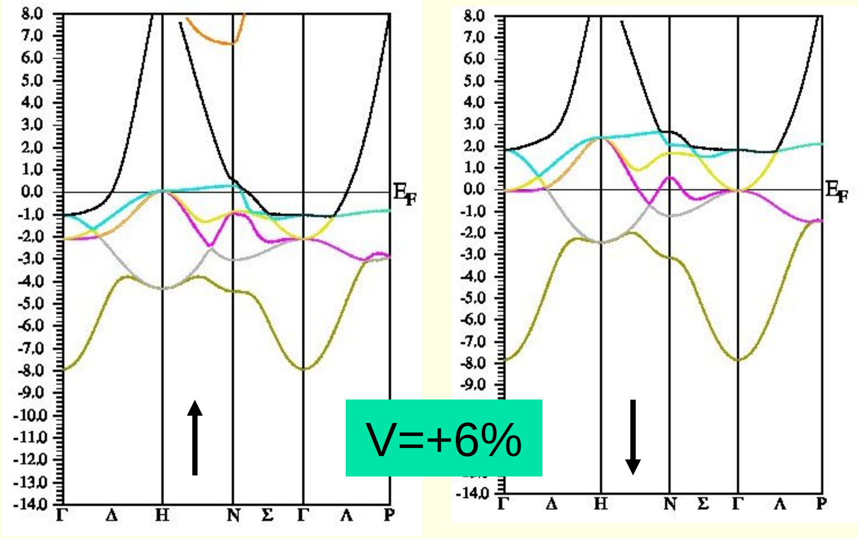
- Magnetism: bcc Fe (a_0=2.86 Å)
  - *setrmt: 3%; 5000k; spin-polarization:yes, use RKmax=7, then 8*
  - *do a volume optimization (-6, -3, 0, 3, 6 %) (activate runsp_lapw instead of run_lapw !)*
    - check equilibrium volume, :MMT as function of volume



```
--- MMTOT ----------- in 5 files:
Fe_vol___0.0_rk8_5000k.scf::MMTOT: 2.21
Fe_vol___3.0_rk8_5000k.scf::MMTOT: 2.26
Fe_vol__-3.0_rk8_5000k.scf::MMTOT: 2.16
Fe_vol___6.0_rk8_5000k.scf::MMTOT: 2.31
Fe_vol__-6.0_rk8_5000k.scf::MMTOT: 2.13
```

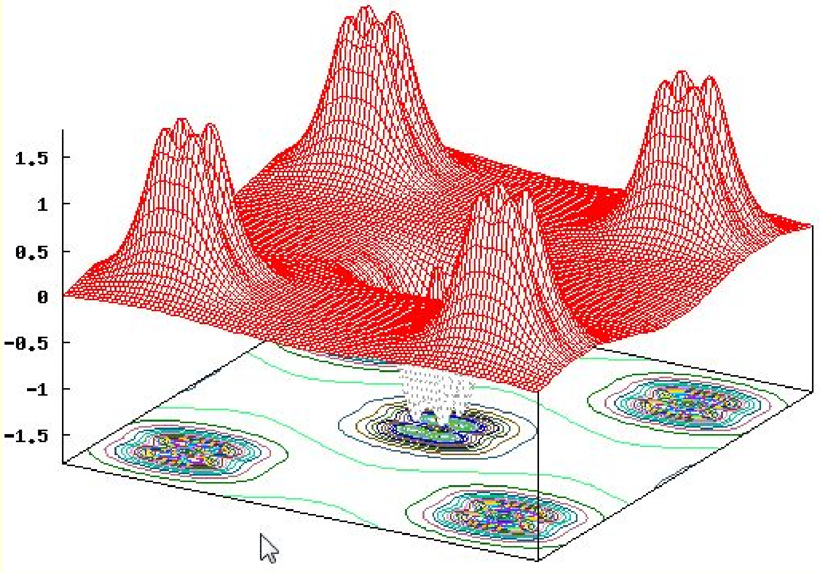
- *compare bandstructure and DOS for large/small volumes (restore_lapw for desired volume; x lapw0 "recreates" potentials, adjust EF in case.insp)*





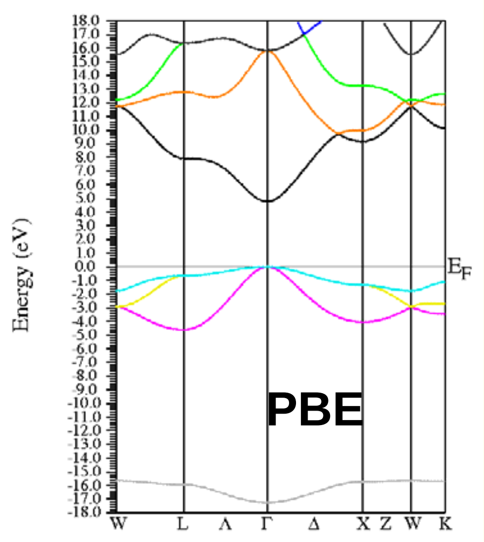
Exercise 6: antiferromagnetic calc.

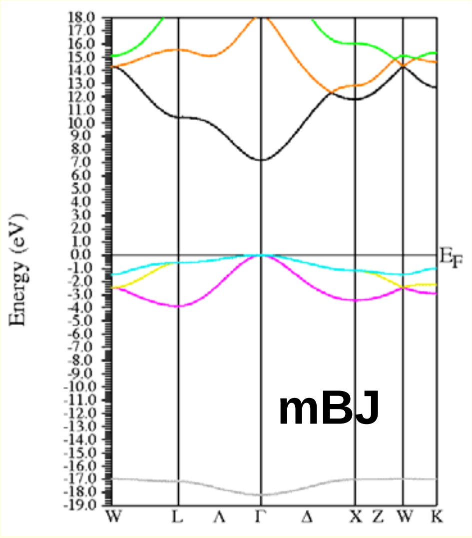
- Antiferromagnetism: bcc Cr (a_0=2.885 Å) (use 5000k, -cc 0.001)
  - *try 2 different calculations:*
  - *ferromagnetic solution (bcc cell with 1 Cr)*
  - *antiferromagnetic calculation (P cell with Cr1 and Cr2 (at 0.5,0.5,0.5))*
    - choose up/dn for the two Cr atoms when creating case.inst
    - for afminput your symmetry operation is "identity+(0.5,0.5,0.5)"
  - *is FM or AFM Cr more stable? (:ENE)*
  - *is FM stable at all ? check moments (MMI001: what "means" 0.000x ???)*
  - *plot spin-densities in the (110) planes*
    - do lapw2 for both spins
    - observe "spatial localization"
    - t_{2g}-asymmetry
    - negative spin-density in interstitial
      - where does it come from ?
      - compare :QTLxxx

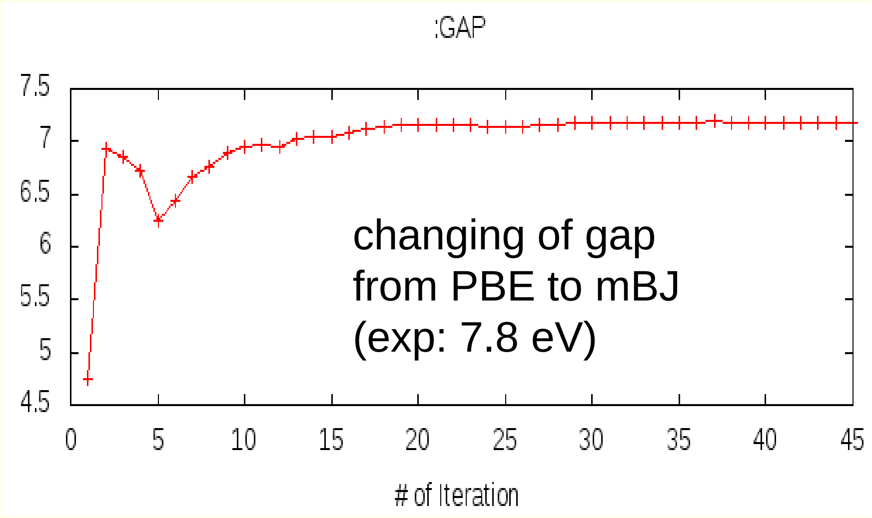


Exercise 7: band gaps of MgO

- MgO (NaCl, a=7.96 bohr; default initialization; scf-cycle)
  - *PBE: check the gap (:GAP from "anaylysis"),*
    - plot a band structure in PBE (E-range from -19 to 18 eV)
  - *TB-mBJ:*
    - save the PBE calculation, execute:
      - init_mbj_lapw (in utils) „phase 1" of the initialization (see also in the UG 4.5.9)
      - run_lapw -NI -i 1
      - rm *.bro*
      - init_mbj_lapw „phase 2", use original mBJ parameters
    - run scf cycle (note, it may not converge in 40 cycles, submit another run with -NI option)
    - monitor the change of the :GAP
    - plot a band structure (fcc) and compare with PBE



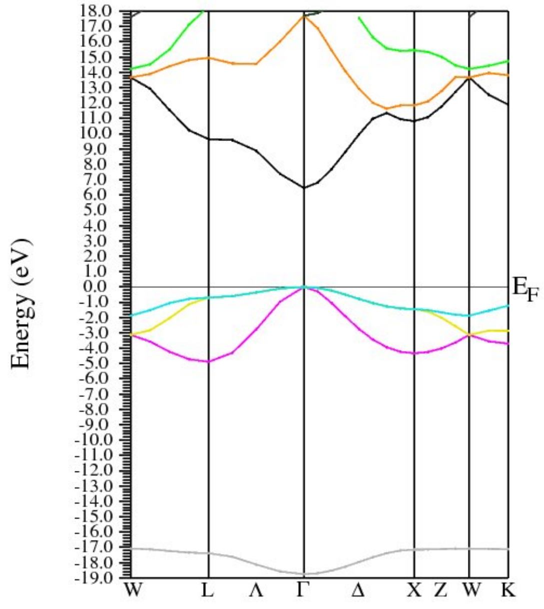




changing of gap
from PBE to mBJ
(exp: 7.8 eV)

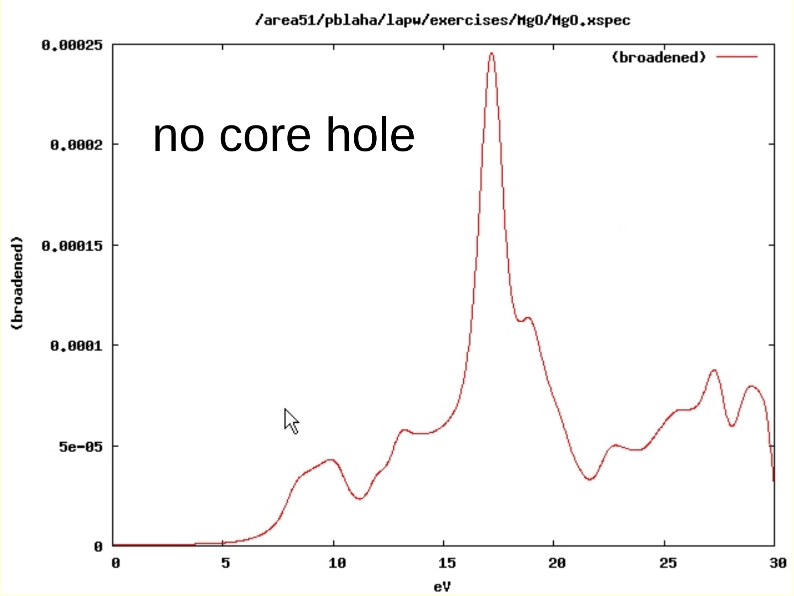
Exercise 7: continued …

- Perform a hybrid-DFT calculation using YS-PBE0
  - create a new case, perform a PBE calculation and save the results.
  - the setup for hybrid-calculations can be made in w2web (Utils/init_hf_lapw), or in a terminal-window using „init_hf_lapw“. (More details are given in the UG 4.5.8)
    - Select NBAND=12 (case.inhf)
    - and a 4x4x4 / 4x4x4 k-point mesh (no reduction)
  - scf cycle with **-hf -p -scratch ./** (insert 2 lines with **1:localhost** into **.machines**)
    - we do this in k-parallel since it will take more time, alternatively we could also use a „reduced“ hf-k-mesh, see UG
  - monitor the change of the :GAP and compare it with mBJ and exp. gaps (only every 2nd value is from HF !)
  - plot a band structure:
    - only the k-mesh selection can be done in w2web, then open a terminal and change into the proper directory
    - run_bandplothf_lapw -p
    - cp $WIENROOT/SRC_templates/case.insp case.insp (insert E_F and increase the plotting energy range).
    - x spaghetti -hf -p

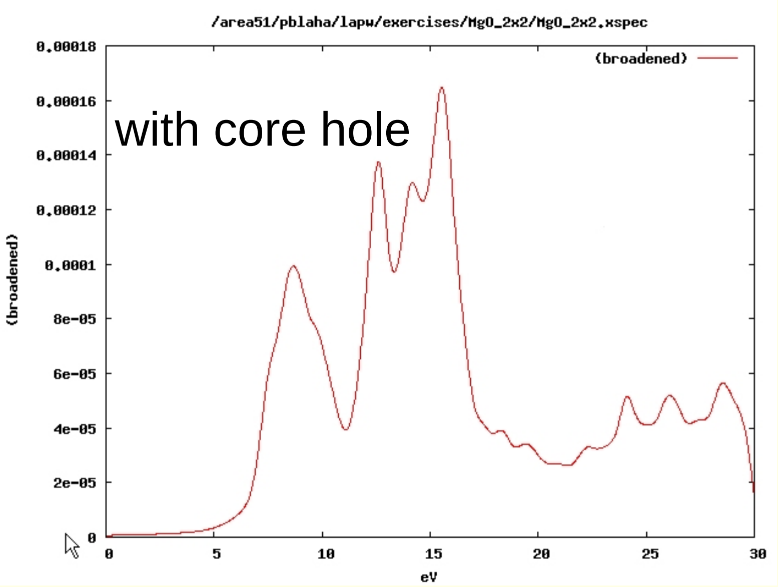


Exercise 8: Mg K-XAS in MgO

- MgO (NaCl structure, a=7.96 bohr; default initialization with 1000 k-points; scf-cycle)
  - *XSPEC task: larger EMAX in MgO.in1; select in MgO.inxs: Mg-K ABS from 0-30 eV, vary broadening)*
- Supercells: MgO 2x2x2 FCC-supercell for core-hole simulation
  - *create new "session", copy MgO.struct into new directory*
  - *x supercell; (specify proper struct-filename, 2x2x2, F-lattice)*
  - *cp supercell-struct file to correct name "case.struct"; "**label**" 1st atom (Mg → Mg1)*
  - *init_lapw (with 200k, RKmax=6.5)*
  - *edit case.inc (remove a core electron from 1st atom)*
  - *edit case.in2 (add one valence electron)*
  - *run_lapw (for bigger calc. use -it and compare timings for 1st and later iterations!)*
  - *edit case.in2 (remove extra valence electron)*
  - *XSPEC task for Mg-K XAS (see above)*


no core hole

Mg-K XAS


with core hole

Exercise 9: LDA+U calculations (command line)

- NiO: NaCl structure, A-type AFM along [111]:
  - *This exercise should be done WITHOUT w2web in a terminal window !*
  - *cd ~/WIEN2k; mkdir NiO; cd NiO*
  - *makestruct*   *# this creates init.struct*
    - NiO: F-lattice, a=b=c=4.195 Ang, α=β=γ=90°
    - Ni (0, 0, 0), O (0.5, 0 , 0)
    - setrmt 3%
- NiO supercell for A-type AFM along [111] (alternating ferromagnetic planes
  - *octave*
    - helpstruct   # lists all structeditor commands
    - help loadstruct   # gives help for specific command
    - s=loadstruct(“init.struct”)   # load fcc NiO struct file
    - sc=makeprimitive(s);   # convert FCC into primitive R cell
    - sr=makesupercell(sc,[1 1 0; 0 1 1; 1 0 1]); # create supercell (110 vectors)
    - showstruct(sr)   # view the structure
    - savestruct(sr,“NiO.struct“)
    - quit

Exercise 9: LDA+U calculations

- *edit NiO.struct and label atoms „Ni1" and „Ni2" (use overwrite mode, don't „insert" 1 and 2 !!!) # this labels spin-up/dn Ni atoms*
- *x sgroup # determines SG, makes O atoms equivalent*
- *cp NiO.struct_sgroup NiO.struct # use the new struct file*
- *xcrysden --wien_struct NiO.struct # visualize and understand the structure*
  # switch convential/primitive cell; R-cell with (a/√2; a/√2; 2 a √3)
- *instgen -ask # generates non-default NiO.inst: put Ni1: up; Ni2:dn; O: nm*
- *init_lapw -b -sp # initialize with all defaults (check init_lapw -h)*
- *runsp_lapw # scf-calc. with all defaults (PBE)*
- *save_lapw NiO_pbe # save the calculation*
- *x lapw2 -up -qtl; x lapw2 -dn -qtl # calculate partial charges for DOS*
- *configure_int -b total 1 tot,d 2 tot,d 3 tot,s,p # configure which DOS to calc.,*
  - also possible without batch mode
- *x tetra -up; x tetra -dn # calc. DOS*
- *dosplot2 -up # plot DOS*
- *save_lapw -dos NiO_pbe # save the DOS*

Exercise 9: LDA+U calculations

- GGA+U calculation
  - *x orb; x lapwdm -up*   *# generate default input files*
  - *edit NiO.inorb; edit NiO.indm   #actually, the defaults are ok for NiO*
    - use U=7eV, J=0; search the UG to understand case.inorb/indm
  - *runsp_lapw -orb*   *#scf-calc. with PBE+U*
  - *save_lapw NiO_pbe+u*
  - *calculate and save the DOS as above ….*
- GGA+SO calculations (M=[111], without relativistic LO, Emax=5.0)
  - *initso_lapw*
    - select M=[111], no relativistic LO, Emax=5.0, spin-polarization and accept the new struct file.
  - *runsp –so –orb*
  - *x lapwdm –up –so   # for orbital moment :orb001 in NiO.scfdmup*
  - *save_lapw NiO_pbe+u+so*
  - *calculate and save DOS*

Exercise 9: LDA+U calculations

- TB-mBJ calculation (without SO):
  - *restore NiO_pbe* *# restore pbe calculation*
  - *init_mbj_lapw* *# and follow the instructions on the screen*

- after all scf: compare DOS (total, Ni1, Ni2, O)
  - observe the change in gaps (exp: 4eV) and shift of Ni/O weights
  - compare spin moments (GGA: 1.41; GGA+U: 1.76; GGA+U+SO:1.76;GGA+SO: 1.41μB)
  - compare orbital moments for SO and SO+U calculations (0.12 and 0.09μB)

NiO cont…

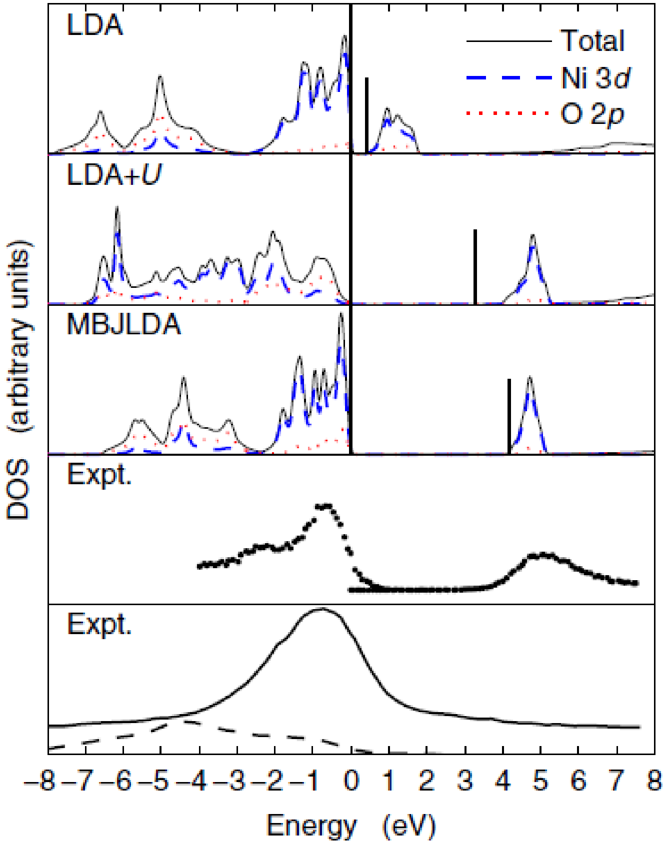
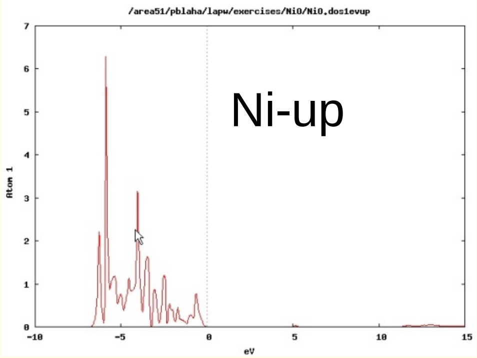
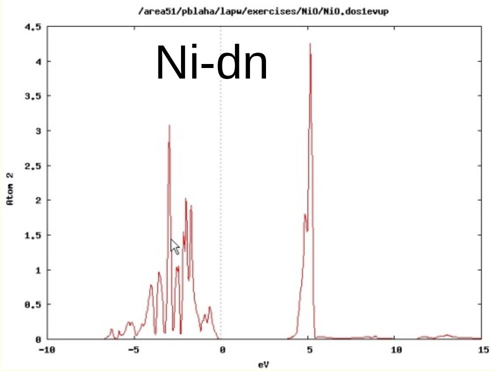


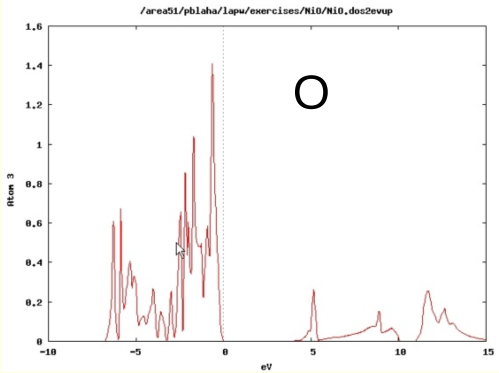
FIG. 2 (color online). DOS of NiO. The vertical bars indicate the end of the fundamental band gap which starts at $E = 0$ eV. The panels labeled “Expt.” show photoelectron [25] (upper panel) and XES [33] [lower panel, Ni (solid line) and O (dashed line) spectra] measurements.

from Tran,Blaha, PRL 102, 226401 (2009)

GGA+U



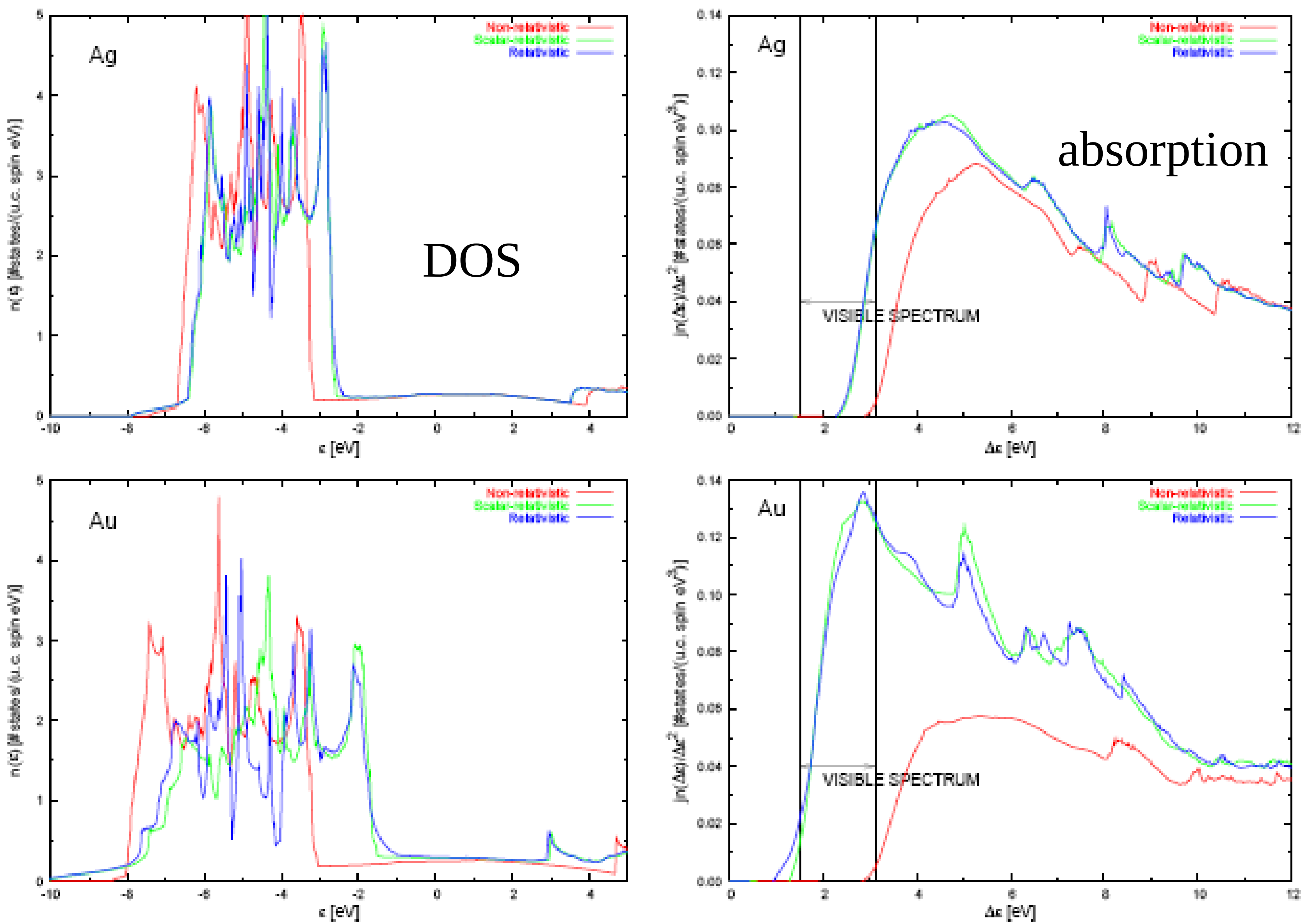




Exercise 10: optical properties

- Optical properties: fcc Al
  - *a_0=4.05 Å*
  - *init_lapw (use 165 **IBZ** k-points only!)*
  - *run_lapw*
  - *calculate optics (as described in the optics lecture, compare with the Al - Fig.)*
    - calculate plasma frequency (case.outputjoint) and dielectric function
    - check your results with respect to k-mesh
      - x kgen (check for about 1000 and 4000 **IBZ**-points)
      - x lapw1
      - x lapw2 –fermi
      - x optic, x joint, x kram
- Optical properties: fcc Ag and Au (both have a_0=4.08 Å)
  - *compare optics without / with spin-orbit coupling (compare with RL)*
    - do NREL (change RELA to NREL in case.struct) first, do the optics
    - do scalar-relativistic calc., do the optics
    - include spin-orbit: run_lapw -so (case.inso **without RLOs** since optic does not support RLOs; put large Emax in case.in1); optics

Ag and Au: a relativistic effect



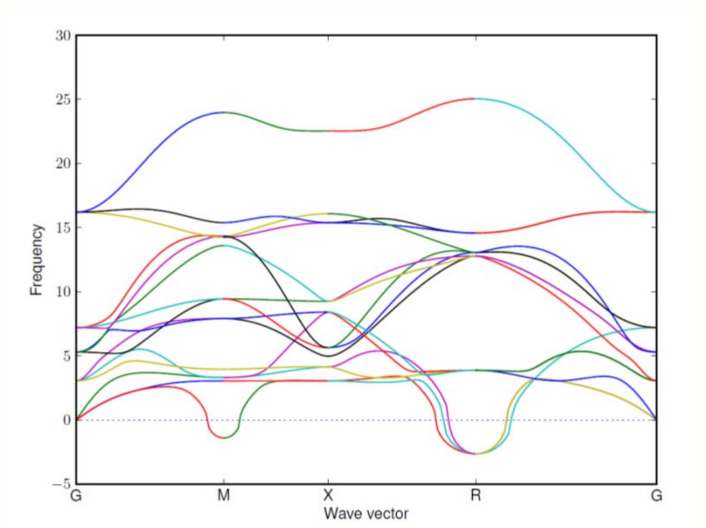
Exercise 11: Phonons of SrTiO$_3$

- This exercise should be done WITHOUT w2web in a terminal window !
- `mkdir SrTiO3; cd SrTiO3;`
- `makestruct`
  - *SrTiO$_3$: SG 221(P m-3m), a=b=c=7.38 bohr, α=β=γ=90°*
  - *Sr (0.5, 0.5, 0.5), Ti (0, 0, 0), O (0.5, 0 , 0)*
  - *setrmt 3%*
- `cp init.struct SrTiO3.struct`
- `init_lapw -b -numk 10 -rkmax 6        # (batch mode)`
- `run_phonopy --wien2k -c SrTiO3.struct -d --dim=“2 2 2”`
- `mkdir 1; mkdir 2; mkdir 3`
- Copy SrTiO3.structS-001, SrTiO3.structS-002 and SrTiO3.structS-003 in 1,2 and 3
- Do the same for directories 1, 2 & 3 (open 3 terminals and do it in parallel):
  - *`cd 1`*
  - *`mv SrTiO3.structS-001 1.struct`*
  - *`init_lapw -b -numk 10 -rkmax 6        #(batch mode)`*
  - *`run_lapw -fc 0.1`*
  - *`cp 1.scf ..`*

Phonons continued

- run_phonopy --wien2k -f 1.scf 2.scf 3.scf
- create band.conf with editor, containing the following information:
  - ATOM_NAME = Sr Ti O
  - DIM = 2 2 2
  - PRIMITIVE_AXIS = 1.0 0.0 0.0 0.0 1.0 0.0 0.0 0.0 1.0
  - BAND = 0 0 0 1/2 1/2 0 0 1/2 0 1/2 1/2 1/2 0 0 0
  - BAND_LABELS = G   M X R G
  - BAND_CONNECTION = .TRUE.
- run_phonopy --wien2k -c SrTiO3.struct band.conf –p
- save with: run_phonopy --wien2k -c SrTiO3.struct band.conf –p –s #(band.pdf)
- your result should be like:

phonons are unstable because $SrTiO_3$ has distorted, tetragonal structure at low temperatures



Exercise 12: Ga-NMR in BaGa$_4$

- This exercise should be done WITHOUT w2web in a terminal window !
- `mkdir BaGa4; cd BaGa4`
- `makestruct` (and type in the following information)
  - *BaGa$_4$: SG 139 (I4/mmm), a,a,c= 4.566 4.566 10.775 Ang*
  - *Ba (0,0, 0), Ga1(0.5,0, 0.75), Ga2 (0,0, 0.38)*
- `cp init.struct  BaGa4.struct`
- `init_lapw -b -numk 10000 –fermit 0.004` (batch mode)
- edit .machines (insert 2 lines with 1:psi3X)
- `run_lapw -p -fc 1 -cc 0.0001;` `save_lapw rkm7_10k_4mry`
- `tail *scf` and verify that the forces are “small” (no struct opt. necessary)
- `x_nmr_lapw -mode in1` (and view the resulting *in1c_nmr file)
- `x_nmr_lapw –p –metal`
  - *check BaGa4.outputnmr_integ for σ_{iso} of both Ga atoms*
  - `grep :EFG002 *scf`
  - `grep :EFG003 *scf`

- R.Laskowski et al., J. Phys. Chem. C 2017, 121, 753−760
- * These calc. will take some time, continue next page while run/x_nmr is running

NMR continued ..

- mkdir spin; cp BaGa4.struct spin/spin.struct; cp .machines spin; cd spin
- instgen_lapw –nm; init_lapw –b –sp –numk 10000 –fermit 0.004
- runsp_c_lapw –p;   save non-magnetic
- cp $WIENROOT/SRC_templates/case.vorbup_100T spin.vorbup (and for dn)
- runsp_lapw –p –orbc –cc 0.000005; save_lapw rkm7_10k_4mry
- grepline :hff002/3 ´rkm*scf´ 3 σ_c=HFF*1000 (for a 100T field)
- compare with experiment: (F.Haarmann et al. Chem. Eur. J. 2011, 17, 7560 – 7568)
- cp $WIENROOT/SRC_templates/case.indm spin.indm;
- edit *indm: set for atom 2 and 3, 3 l values, l=1,2,3; and 3 5 in last line
- x lapwdm –p –up/dn; cat *scfdmup/dn; $\sigma_{sd}=(tot_{up}-tot_{dn})*10000$

case	V_{zz}(exp)	V_{zz}(th)	δ_{iso}(exp)	δ_{iso}(th)
Ga1	5.99		3010	
Ga2	1.20		840	

- $\sigma_{iso}(th)= \sigma_{orb} - \sigma_c - \sigma_{sd}$
- *Estimate $\delta_{iso}(th)=(\sigma_{itot}th)-\sigma_{ref}(th))$; estimate $\sigma_{ref}(th)$ to obtain "best" agreement with exp. (usually one would either calculate the reference compound or do several Ga compounds)*
- *In metals the results are **very** sensitive to k-mesh and smearing and careful convergence are necessary (up to 1 000 000 k-points).*