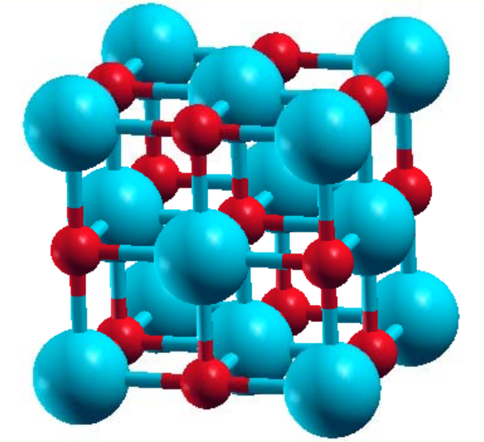
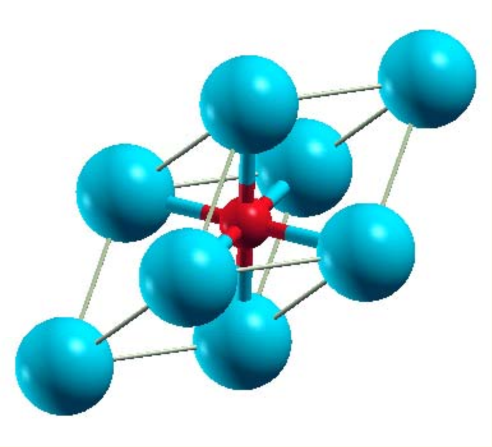
Exercises:

- In the following you find some suggestions for exercises, which teach you various tasks one may perform with WIEN2k.
- 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 !!
- Account information (username/pw): kursXX / wien2k
  - *(for XX put the last 2 numbers shown on your pc)*

Exercise 1: Getting started:

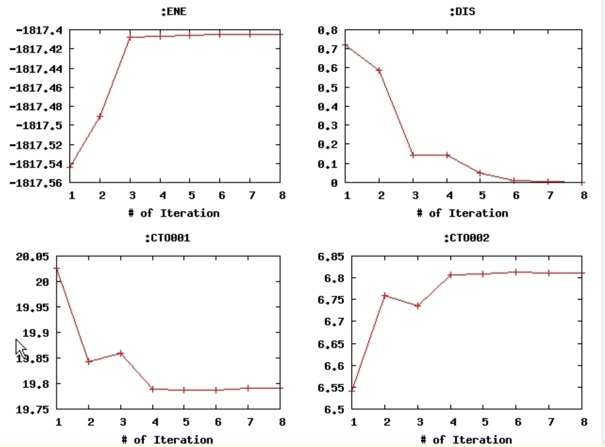
- i) Open a terminal window.
- ii) Start w2web (accept all defaults, specify account (kursXX/wien2k)
- iii) Connect with firefox to w2web as indicated on the screen of ii)
- iv) Try the "quick-start" example for **TiN** (similar to TiC in the UG)
  - *Generate structure (a=4.235 Ang; reduce RMT by 1%)*
  - *view structure with Xcrysden (switch from primitive to conventional cell)*



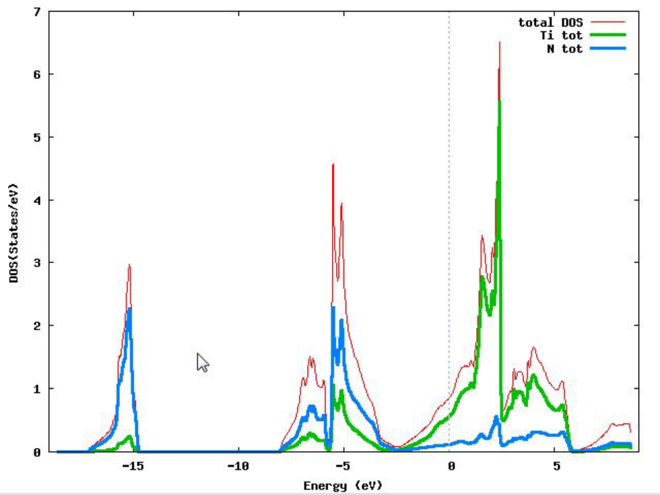


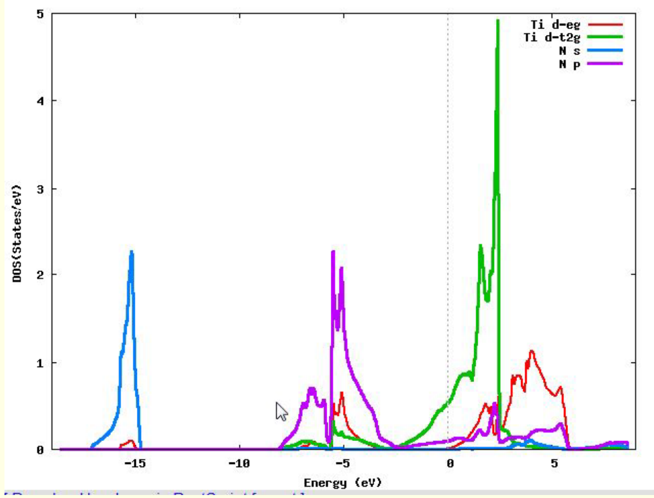
  - *init_lapw (use defaults, 1000 k-points)*
  - *scf-cycle (run_lapw, use defaults; monitor “STDOUT” and “dayfile”)*
    - How many iterations did you need ? How long took a single scf-iteration ?

TiN continued

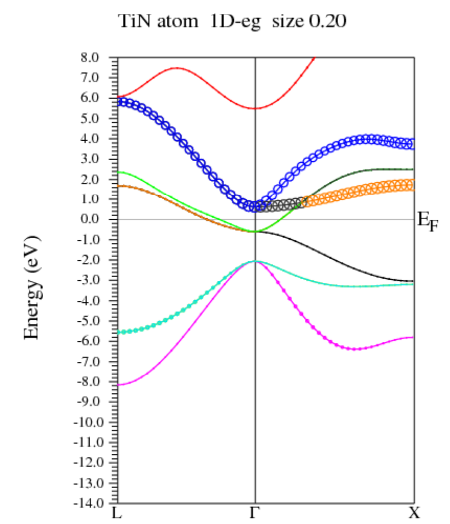


- *utilities: analyse*
  - (:ENE, :DIS, :CTO) graphically
- *utilities: save_lapw (use as save-name: "TiN_exp_pbe_rk7_1000k")*
- *DOS (plot 7 cases: total + Ti-tot + N-tot and Ti-eg + Ti-t2g + N-s + N-p)*





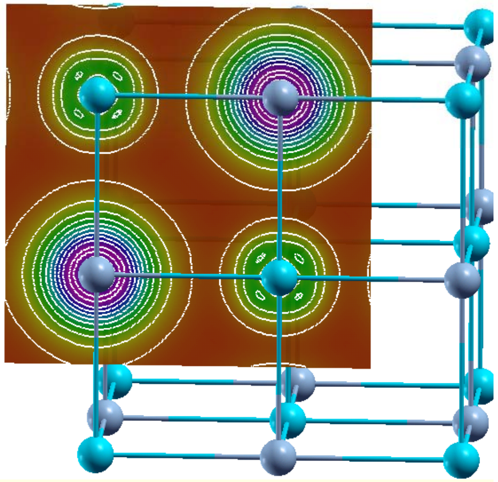
- *bandstructure (along L-Gamma-X with "character plotting") (identify "t2g-" and "eg-" bands)*



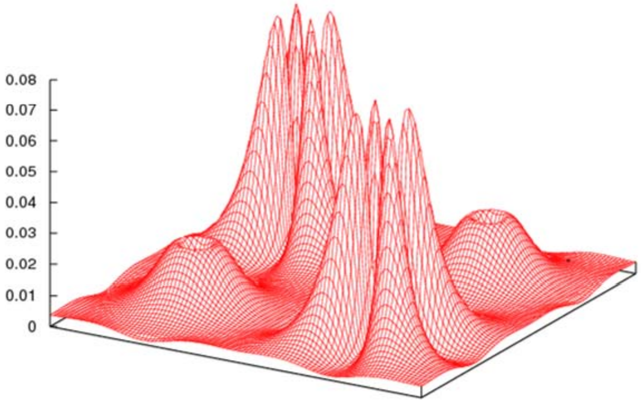
TiN continued ...

- *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 "t2g-anisotropy" around Ti)
  - densities of the "N-p" and "occupied Ti-d-band" (get the corresponding E-intervals from DOS-plots (in Ry!), check UG how to modify TiN.in2 in order to obtain the density in a certain E-interval (search for "case.in2"); observe the eg and t2g asymmetry around Ti and the different N-p "weights", explain the chemical bonding

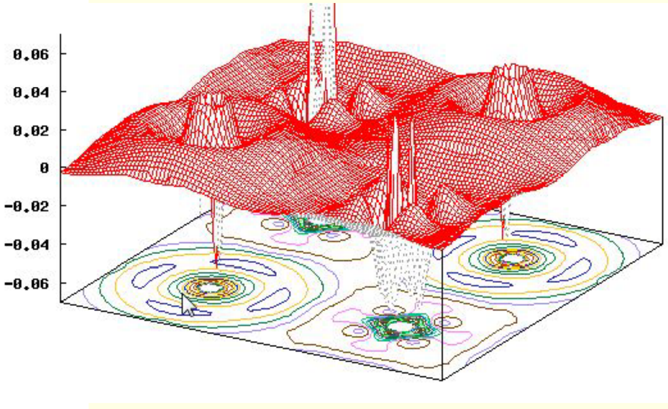
valence ρ



Ti-d band



difference density



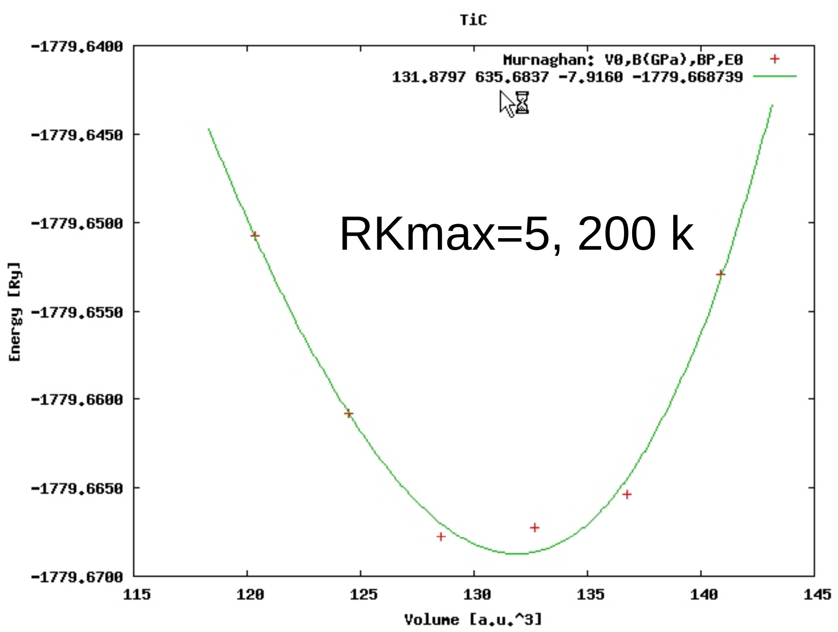
Exercises 2: Testing accuracy: RKmax and k-points

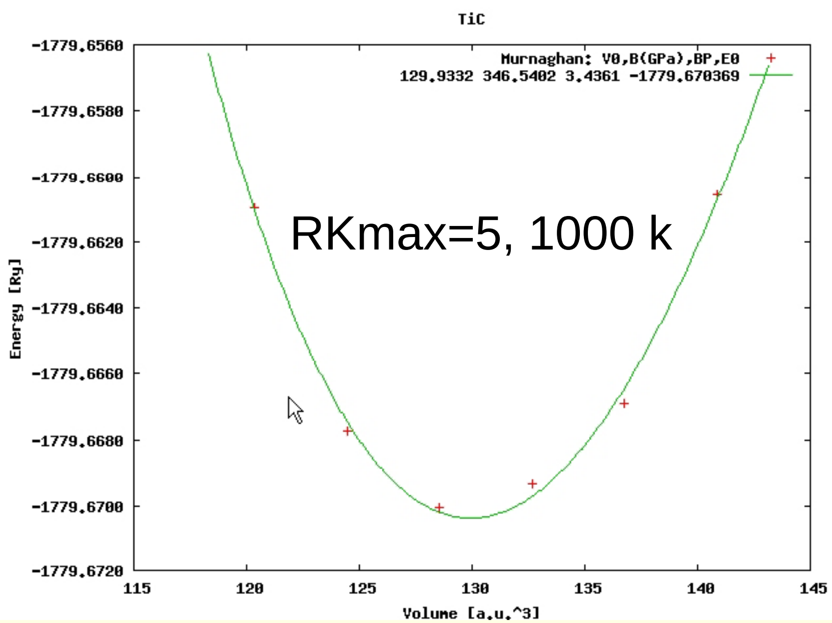
- TiC (fcc, a=4.328 Ang, setrmt – 4%, LDA) and calculate the equilibrium volume ("optimize") using:
  - *(RKmax=5 200 k-points); (RKmax=6.5 200 k); (RKmax=5 1000 k); (RKmax=6.5 1000 k) and (RKmax=8 5000 k)*
- a) run x optimize and generate 6 structures (-12, -9, -6, -3, 0, 3% volume change)
  - *(because of LDA we expect 1-2% smaller lattice parameter (3-8% in volume) than experiment)*
- b) set RKMAX=5 in TiC.in1 and x kgen with 200 k-points
- c) edit "optimize.job". Modify the “run_lapw” and "save_lapw" commands to:
  - `run_lapw –cc 0.001 –ec 0.0001`
  - `save_lapw ${i}_rk5_200k`
- d) run optimize.job, plot the results (using *rk5_200k)
- e) set RKMAX=6.5 in TiC.in1
- f) edit "optimize.job". Uncomment the cp line and modify:
  - `cp ${i}_rk5_200k.clmsum TiC.clmsum` *# Using previously converged densities saves a lot of CPU time!!*
  - *...*
  - `save_lapw ${i}_rk6.5_200k`
- g) repeat step d) (plot the results for “*_rk6.5_200k”)
- h) repeat steps above with proper modifications

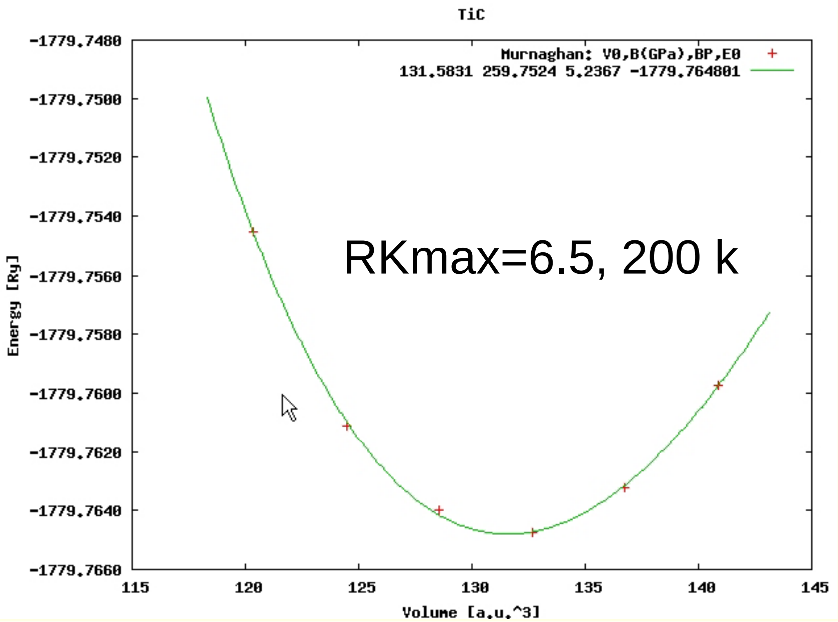
- Find out how RKmax and k-points lead to smooth/non-smooth curves. Estimate good values and compare in particular B and BP (Bulkmodulus and its volume derivative).
- Remember: Depending on the specific property you want to calculate (just a DOS, or Energy-Volume curves, or EFG, or structure optimization with forces,..) and the desired accuracy, the types of atoms, insulator/metal and system size you may need different RKmax and k-point samplings:
  - *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*

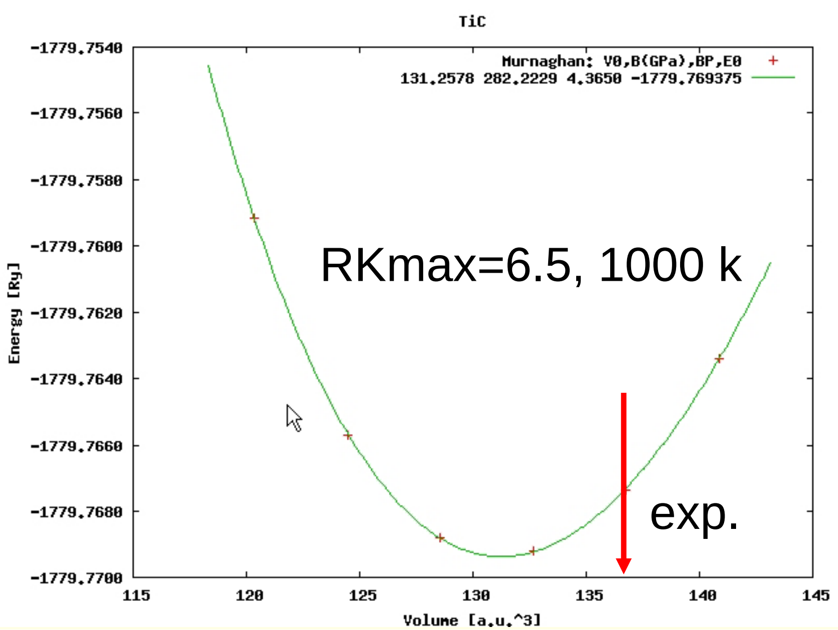
- Remember: Always test your **specific property** for convergence !!

Volume optimization for TiC


RKmax=5, 200 k


RKmax=5, 1000 k

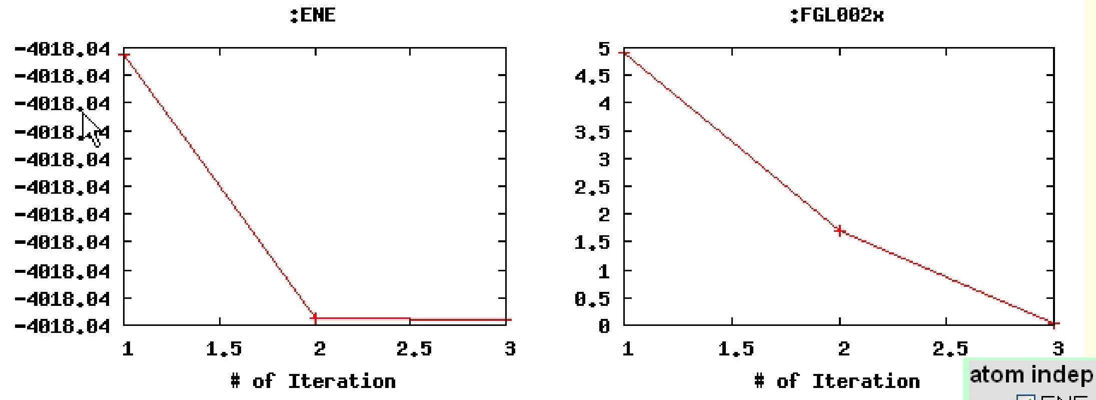

RKmax=6.5, 200 k

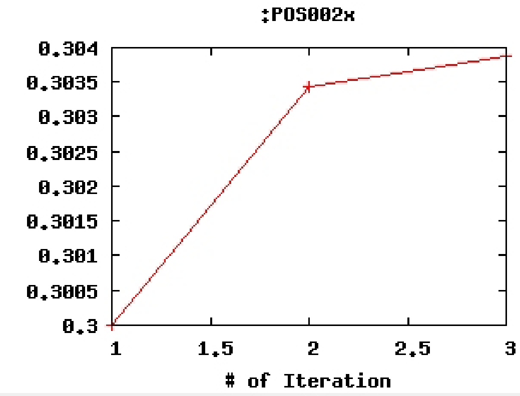

RKmax=6.5, 1000 k

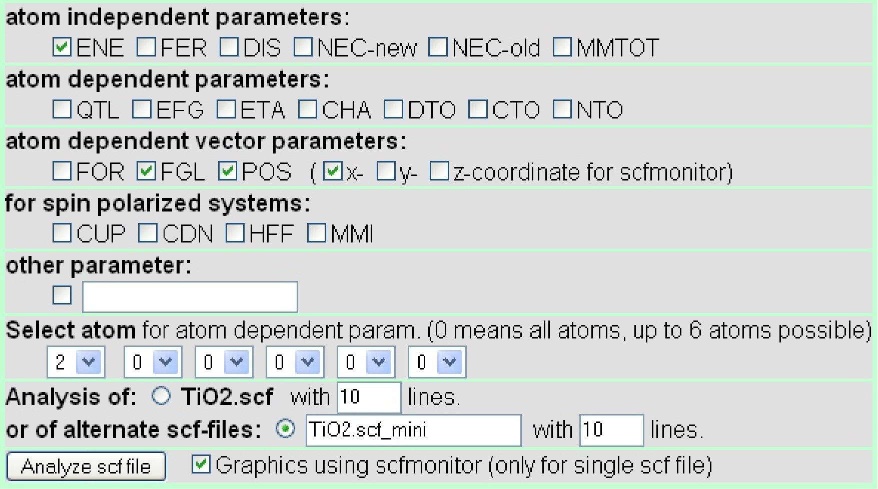
exp.

Exercise 3:

- optimization of positions: rutile TiO_2:
  - *P42/mnm (136), a=b=4.59 c=2.96 Å; Ti(0,0,0)   O(0.3,0.3,0); RMT-2%*
  - *init_lapw: (100k, RKmax=6.5)*
  - *min_lapw (use defaults in case.inM)*
    - analyze :ENE :FGL002x :POS002x in case.scf_mini (exp.pos:0.3045)







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:

☐

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

2 0 0 0 0 0

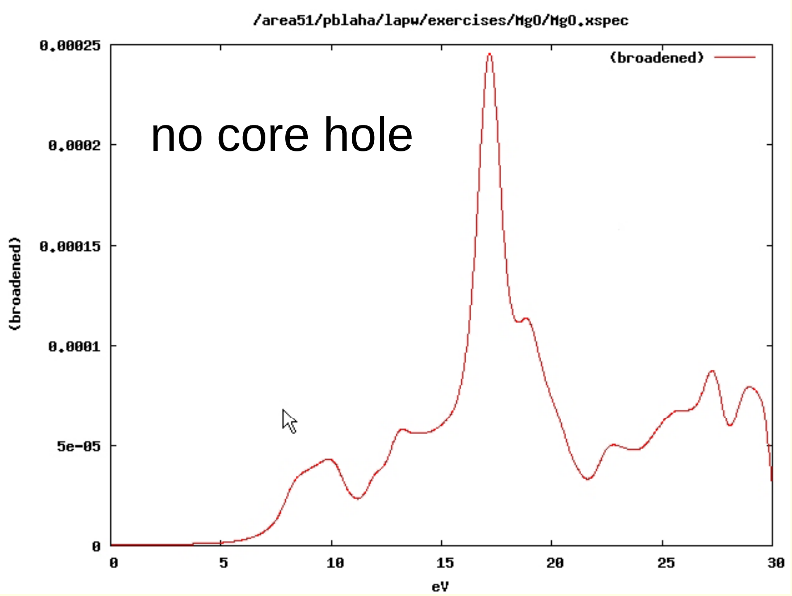
Analysis of: ○ **TiO2.scf** with 10 lines.

or of alternate scf-files: ● TiO2.scf_mini with 10 lines.

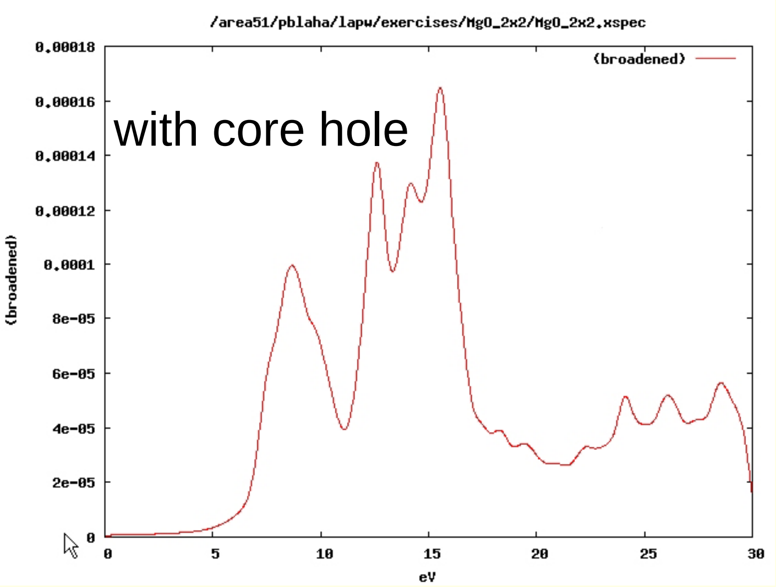
☑Graphics using scfmonitor (only for single scf file)

Exercise 4:

- X-ray emission/absorption spectroscopy
  - *MgO (NaCl structure, a=7.96 bohr; default initialization with 1000 k-points; scf-cycle)*
  - *XSPEC task: Mg-K XAS (select larger EMAX in MgO.in1; spectrum 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 –it (use iterative diagonalization, compare timings for 1st and later iterations!)*
  - *edit case.in2 (remove extra valence electron)*
  - *XSPEC task for Mg-K XAS (see above)*

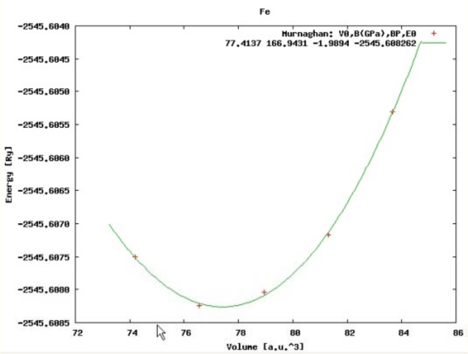


Mg-K XAS



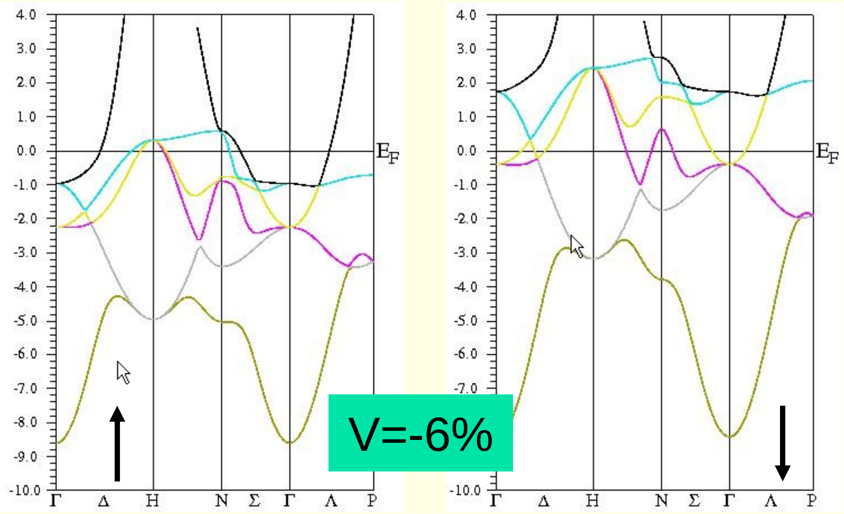
Exercise 5:

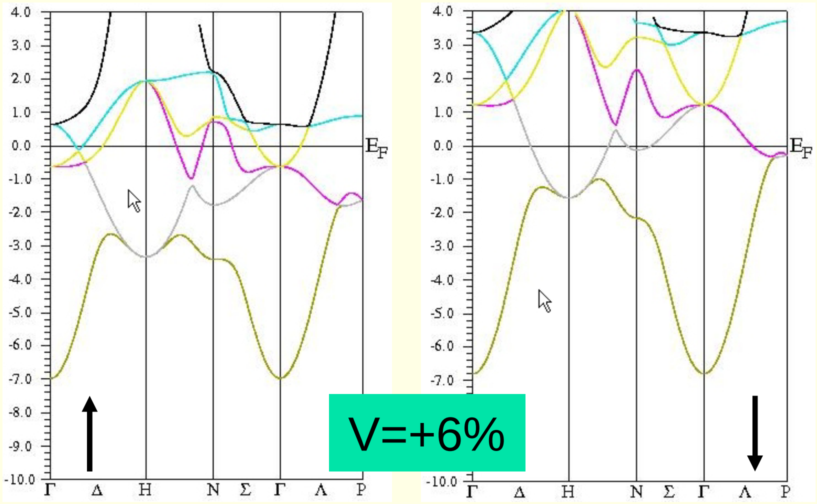
- Magnetism: bcc Fe (a_0=2.86 Å)
  - *setrmt: -3%; 5000k; spin-polarization:yes, use RKmax=7, then 8*
  - *do a volume optimization (-6, -3, 0, 3, 6 %) (activate runsp_lapw instead of run_lapw !)*
    - check equilibrium volume, :MMT as function of volume



```
--- MMTOT ----------- in 5 files:
Fe_vol___0.0_rk8_5000k.scf::MMTOT: 2.204
Fe_vol___3.0_rk8_5000k.scf::MMTOT: 2.258
Fe_vol__-3.0_rk8_5000k.scf::MMTOT: 2.159
Fe_vol___6.0_rk8_5000k.scf::MMTOT: 2.320
Fe_vol__-6.0_rk8_5000k.scf::MMTOT: 2.114
```

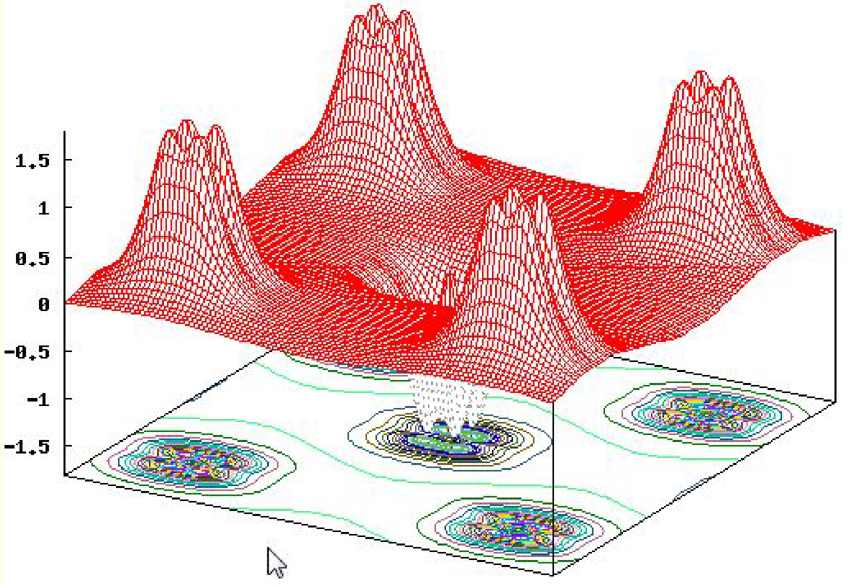
- *compare bandstructure and DOS for large/small volumes (restore_lapw; x lapw0 “recreates” potentials)*





Exercise 5:

- Antiferromagnetism: bcc Cr (a_0=2.885 Å) (use 5000k, -cc 0.001)
  - *try a ferromagnetic solution (bcc cell with 1 Cr)*
  - *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)”
  - *is FM or AFM Cr more stable? (:ENE :-2101.769475 vs. -4203.543208 Ry)*
  - *is FM stable at all ? check moments (MMI001: 0.000 vs. 1.116μ_B; what “means” 0.0 ???)*
  - *plot spin-densities in the (110) planes (observe t2g-asymmetry)*

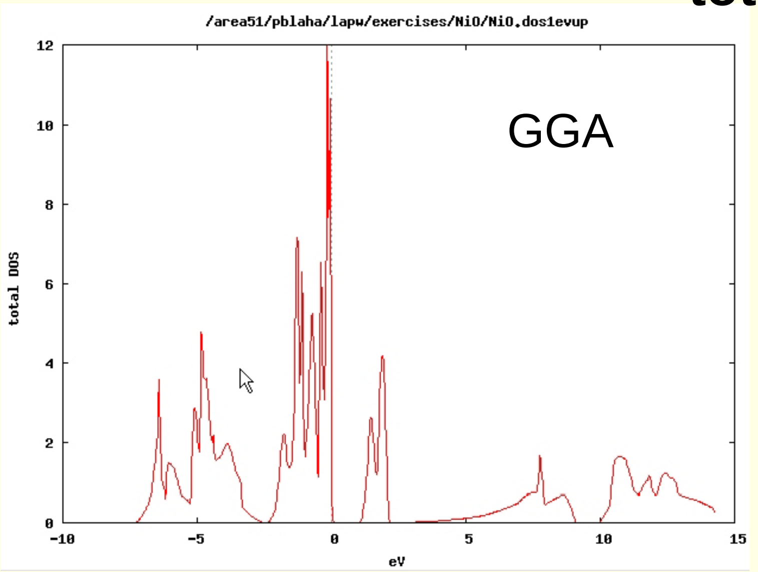


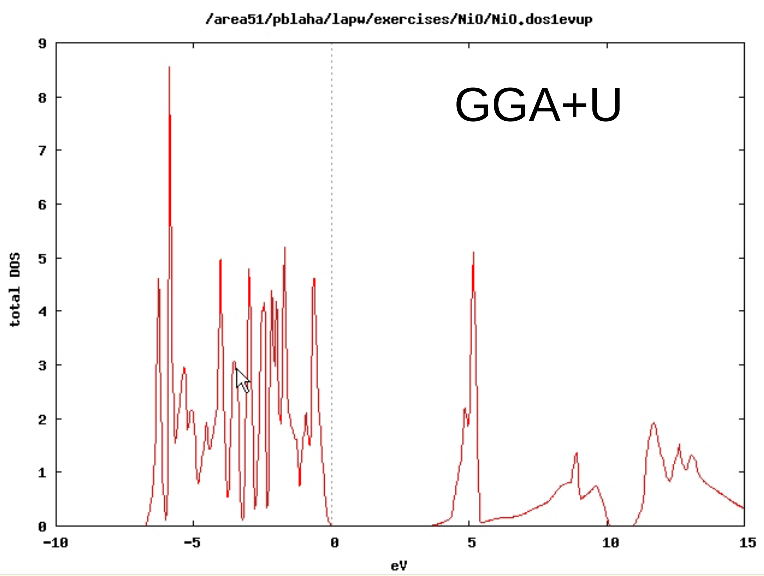
Exercise 6:

- LDA+U: NiO: NaCl structure, A-type AFM along [111]
  - *R-cell: 5.605236 5.605236 27.459934 bohr*
  - *3 non-equivalent atoms: Ni1 (0,0,0), Ni2 (0.5,0.5,0.5), O ±(.25,.25,.25) ("add 2nd position"* ***after*** *first "save_structure"). View and understand the structure (Xcrysden)*
  - *case.inst: flip spin for Ni2, make O "non-magnetic"; use 100k-points*
  - *GGA calculations (save_lapw NiO_gga)*
  - *GGA+U calculations (save_lapw NiO_gga+u)*
    - (use U=7eV, J=0; search the UG to understand case.inorb/indm)
  - *GGA+SO calculations (without relativistic LO, Emax=5.0, new k-mesh!)*
    - after scf: x lapwdm –up –so (for :orb001 in NiO.scfdmup)
  - *GGA+U+SO calculations (cp NiO.indm NiO.indmc)*
  - *compare DOS (total, Ni1, Ni2, O) for GGA and GGA+U*
    - 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: 1.17μB)
    - compare orbital moments for SO and SO+U calculations (0.16 and 0.17μB)

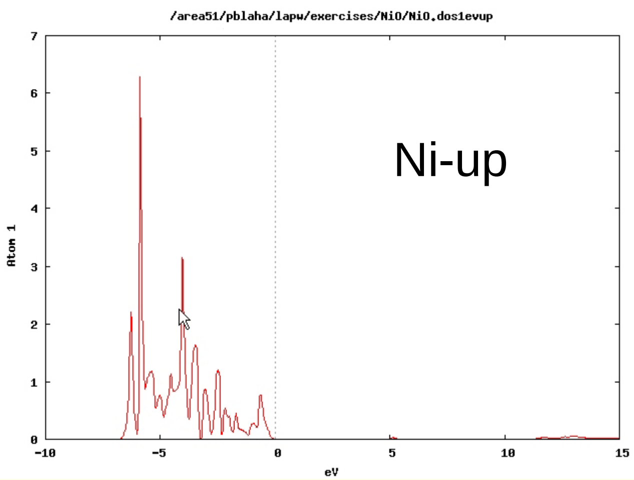
NiO cont...

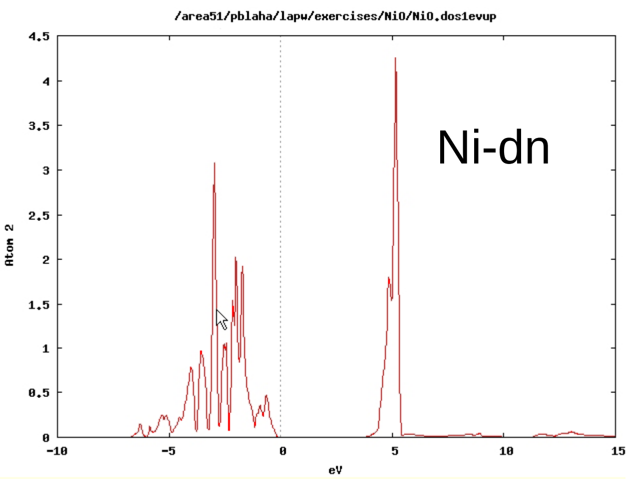
total DOS

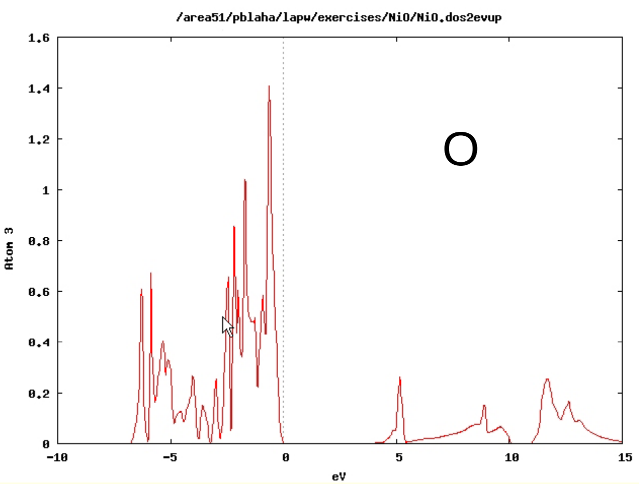




GGA+U







Exercise 7:

- Optical properties: fcc Al
  - *a_0=4.05 Å*
  - *init_lapw (use 165 IBZ k-points only!)*
  - *run_lapw*
  - *calculate optics (as described by C.Ambrosch-Draxl, compare with her 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 Pt
  - *a_0=3.92 Å*
  - *compare optics without / with spin-orbit coupling (compare with CAD)*
    - do scalar-relativistic calc. first including optics
    - init_so (put large Emax in case.in1); run_lapw –so, optics