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 !!

setup of environment

- The description assumes that all software is installed in /opt . (`ls /opt`)
- add wien2k:
  - `cd /opt/WIEN2k`
  - `./userconfig`   *(defines PATH and some variables)*
- add xcrysden:
  - `cd /opt/XCrySDen/1.4.1bin-static`
  - `./xcConfigure.sh`
- add wien2wannier:
  - `cd /opt/wien2wannier`
  - `./link_w2w.sh`
- add path to wannier90
  - `cd ;` *edit* `.bashrc` *(you can use the PASS icon, view/show_hidden_files)*
    - find line : `export PATH=` ... and add at the end of the line
    - ...`:/opt/wannier90-1.2`
- activate environment:
  - `source .bashrc`
- now you are ready to start w2web (define your userid/pw, port-number) and connect via a webbrowser (firefox)

Exercise 1: Getting started:

- i) Open a terminal window.
- 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)
    - *Generate structure (a=4.235 Ang; reduce RMT by 1%)*
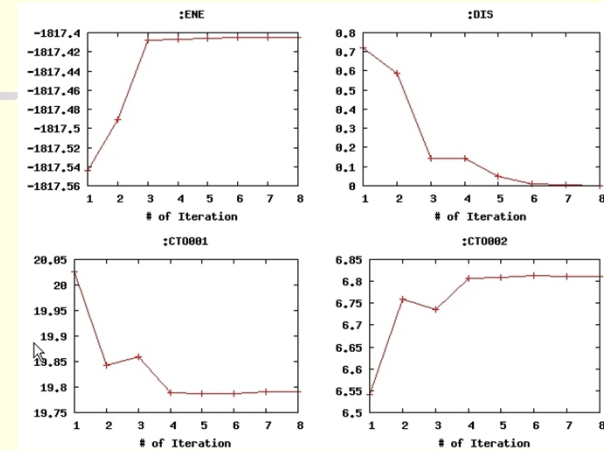   - *view structure with Xcrysden (switch from primitive to conventional cell)*
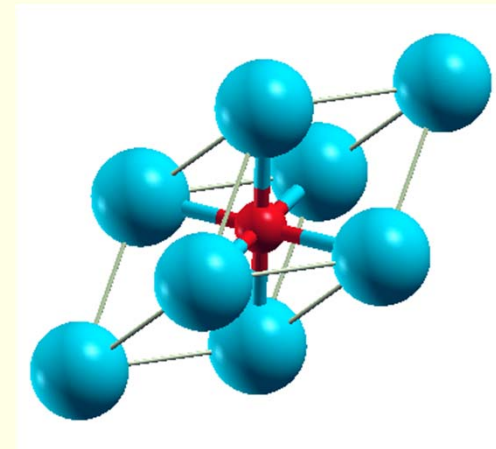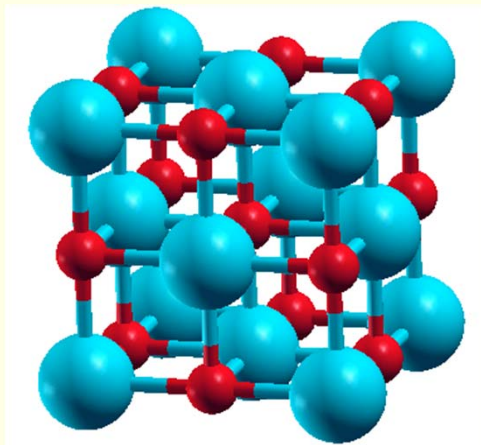
    - *init_lapw (use defaults, 1000 k-points)*
    - *scf-cycle (run_lapw, use defaults; monitor "STDOUT" and "dayfile")*
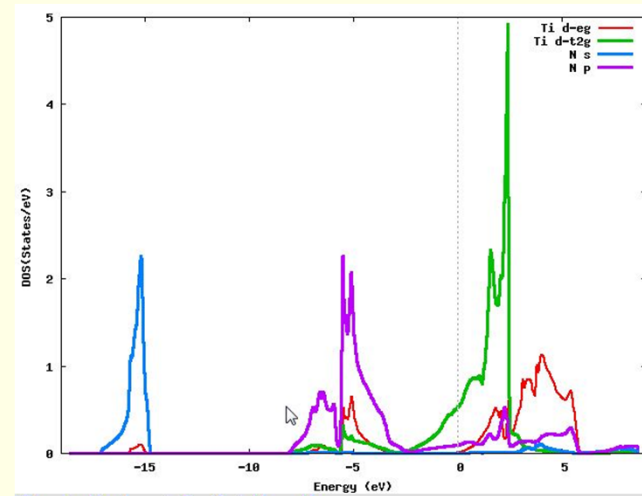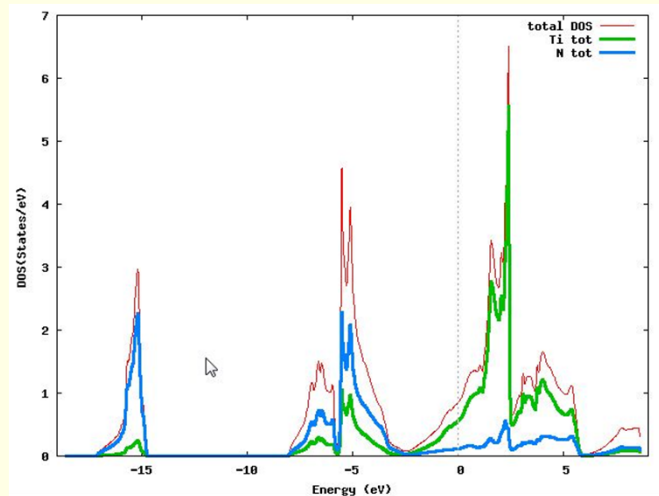   - How many iterations did you need ? How long took a single scf-iteration ?

TiN continued

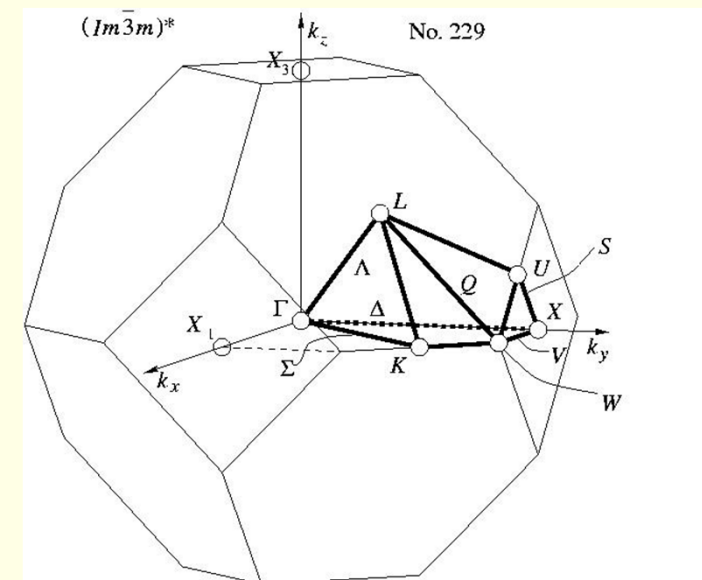- *utilities: analyse*
  - (:ENE, :DIS, :CTO) graphically
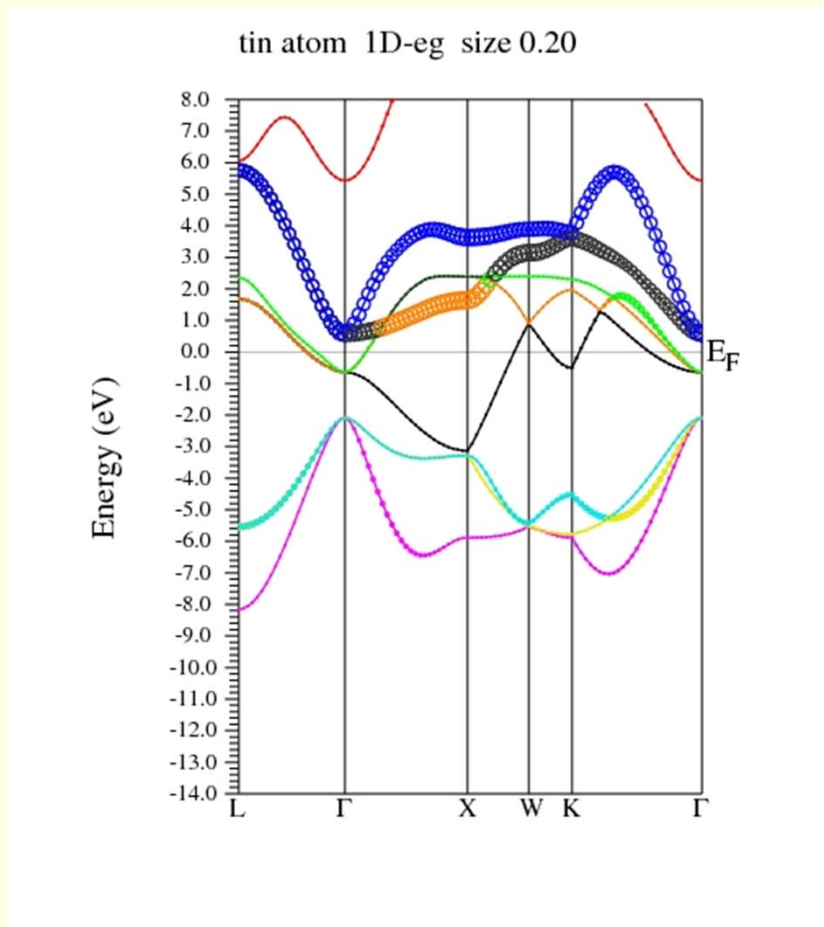
- *utilities: save_lapw (use as save-name: "TiN_exp_pbe_rk7_1000k")*
- *DOS (plot 7 cases: total + Ti-tot + N-tot and Ti-eg + Ti-t2g + N-s + N-p)*

- **bandstructure (along L-Gamma-X-W-K-Gamma with "character plotting")**
  - *use xcrysden (save as „xcrysden.klist"; select „from xcrysden" in next step)*
 - *identify "t2g-" and "eg-" bands*

tin atom 1D-eg size 0.20

- *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

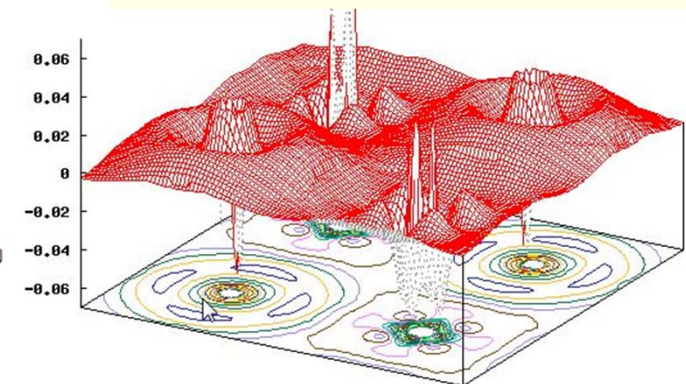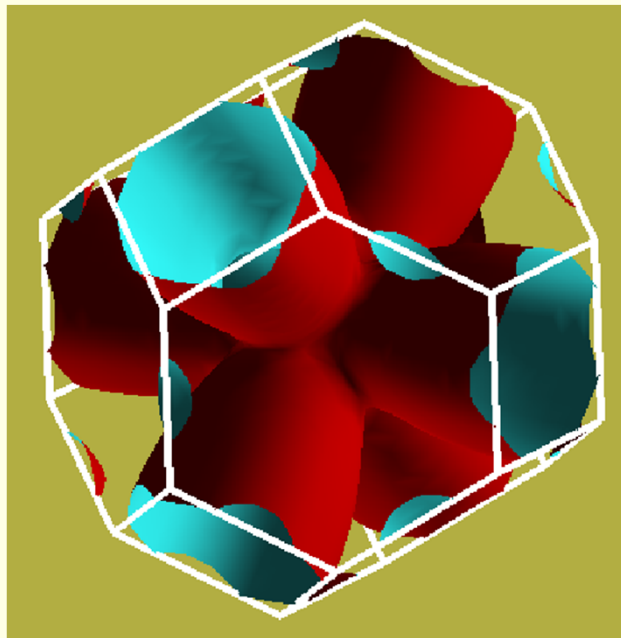valence ρ
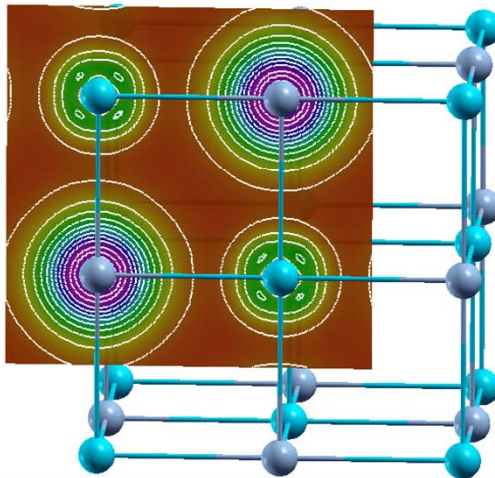
Ti-d band
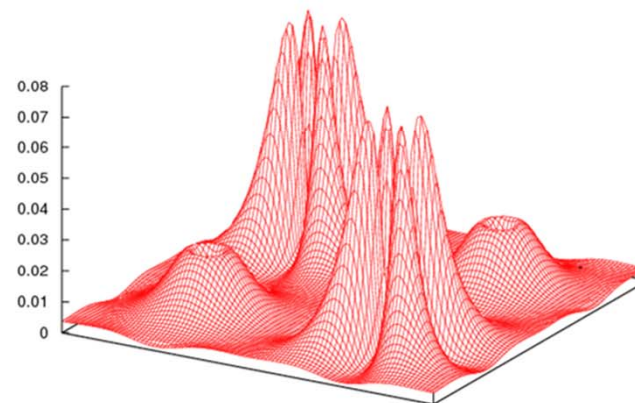
difference density

- *Fermi surfaces*
  - open a terminal, change into the TiN directory and issue:
  - `xcrysden –wien_fermisurface tin.struct`
    - choose a good k-mesh (eg. 10000 points); (DON'T CHANGE to UNIT 5 !!!)
    - plot the FS for all bands (**9**, 10,11) which cross E_F and compare to band structure


 - *for 2D plots there is also a WIEN2k-tool „fsgen" (see UG)*

- 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
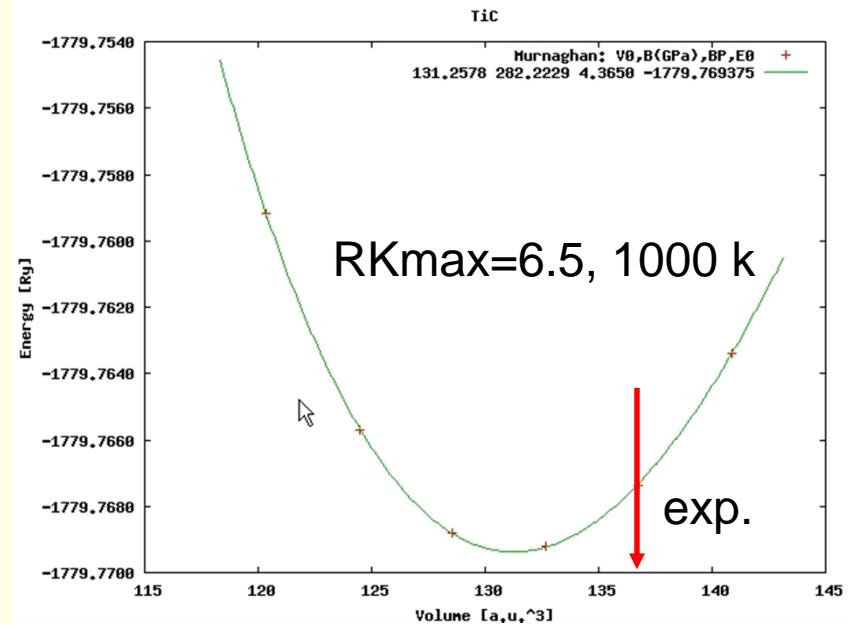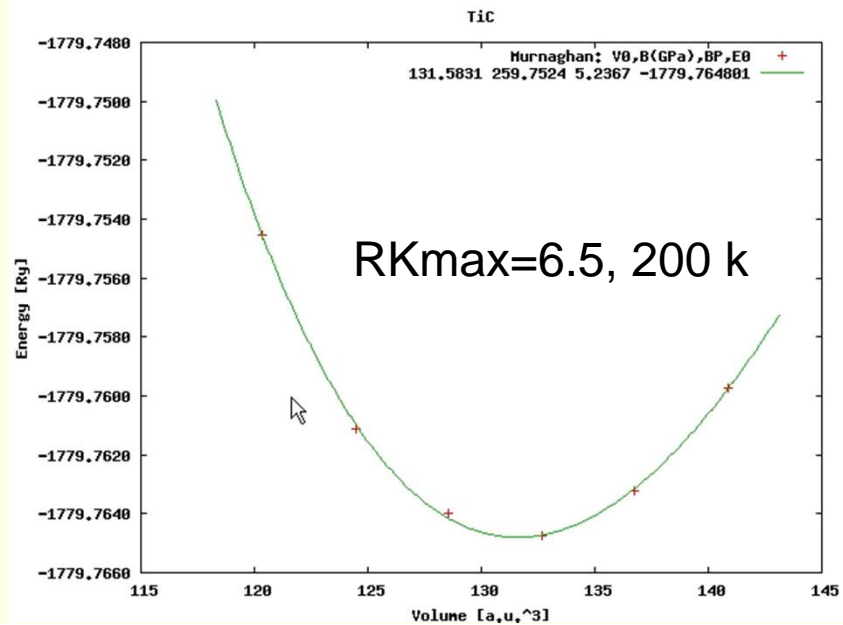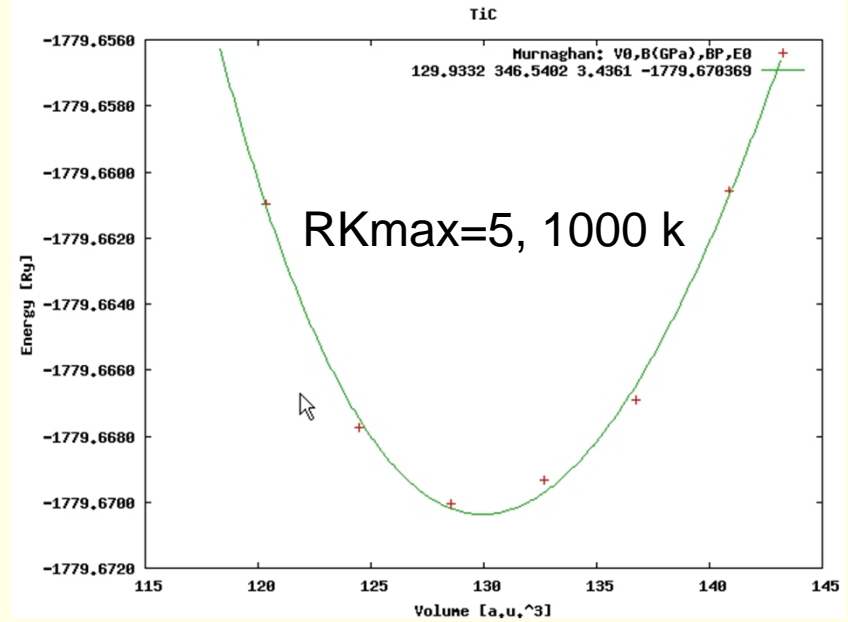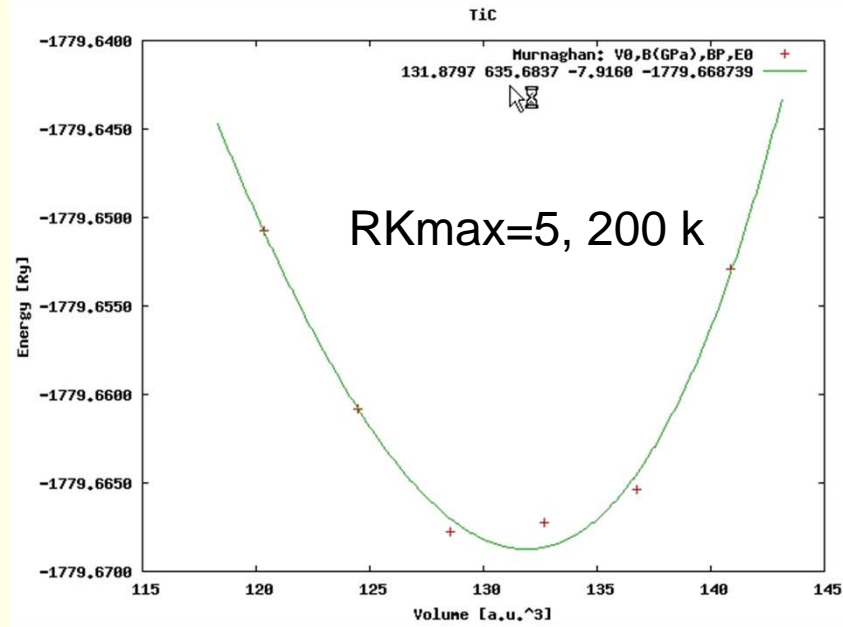
- **create two "cases" (directories) for PORT and MSR1a optimization**
 - *initialize both cases (or copy after init one case to the other and use „rename_files")*
  - *P-3m1 (164), a=b=3.15 c=4.77 Å $\gamma=120^o$; Mg(0,0,0) O(1/3,2/3,**0.22**) H(1/3,2/3,**0.41**); RMT: -7%*
  - *init_lapw -b –numk 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*
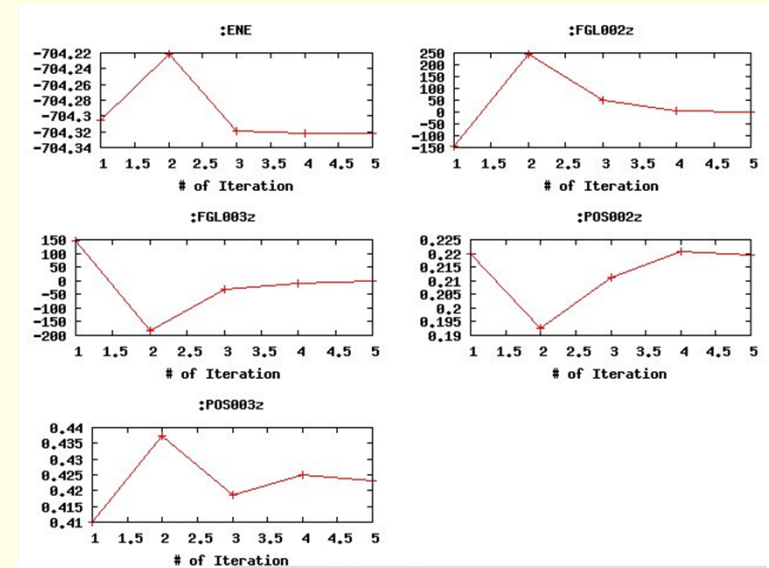
- **minimization using MSR1a:**
  - *run crude scf cycle to come down to „Born-Oppenheimer" surface*
    - run –fc 3; save_lapw case_initial
  - *change MSR1 to MSR1a in case.inm, optimize using:*
    - run –fc 1 –cc 0.0001 –ec 0.00001
  - *analyze* **case.scf** *and find out how many scf cycles you 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.168)*
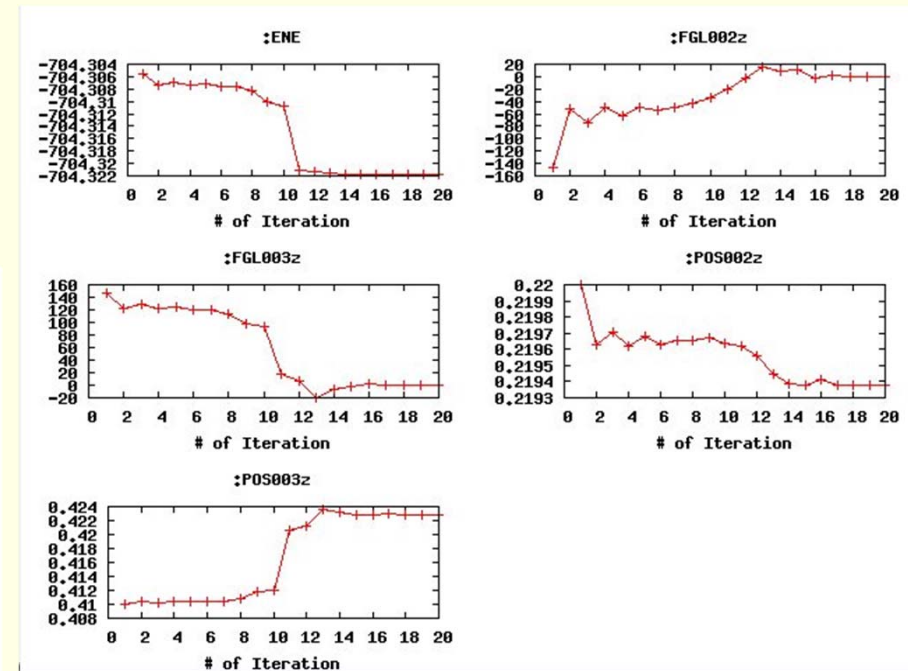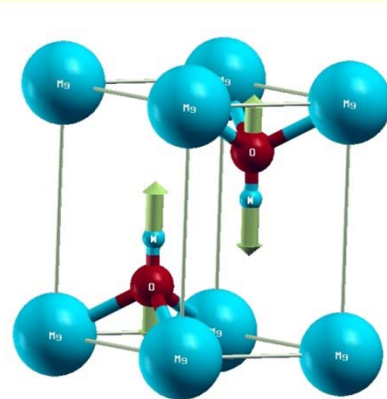
- **MgO** (NaCl structure, a=7.96 bohr; default initialization with 1000 k-points; scf-cycle)
  - *XSPEC task: larger EMAX in MgO.in1; select in MgO.inxs: Mg-K ABS from 0-30 eV, vary broadening)*
- **Supercells: MgO 2x2x2 FCC-supercell for core-hole simulation**
  - *create new "session", copy MgO.struct 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)*

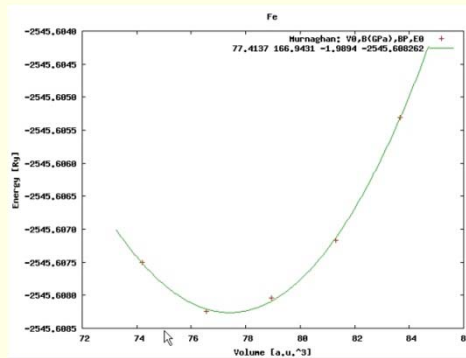no core hole

Mg-K XAS

with core hole
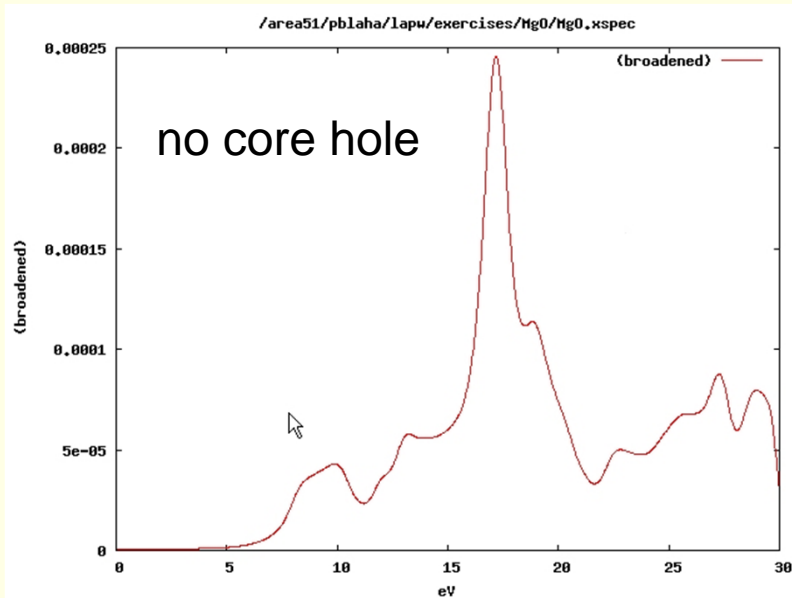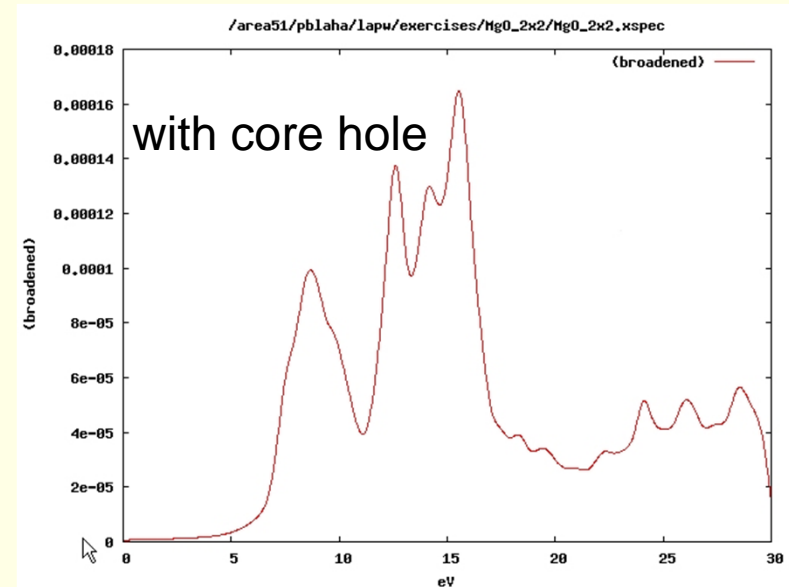
Exercise 5:

- **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
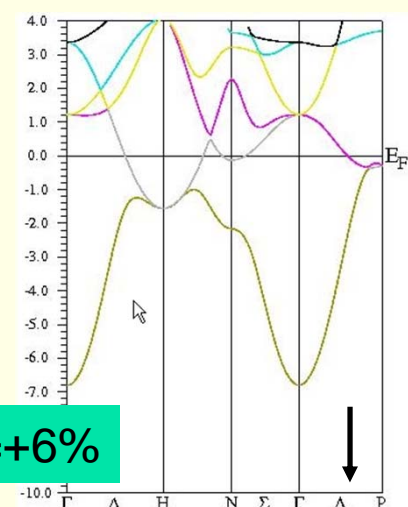

--- MMTOT ----------- in 5 files:
Fe_vol___0.0_rk8_5000k.scf::MMTOT: 2.204
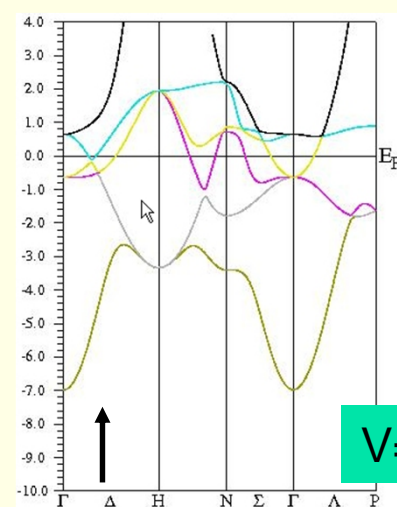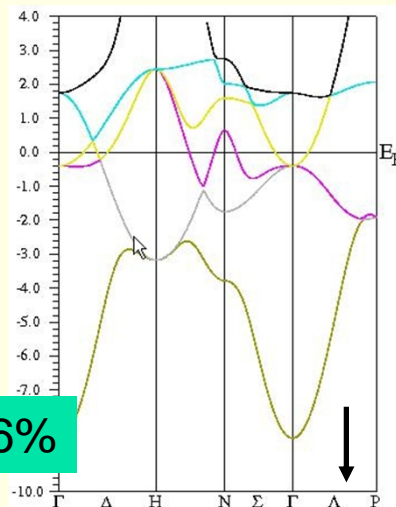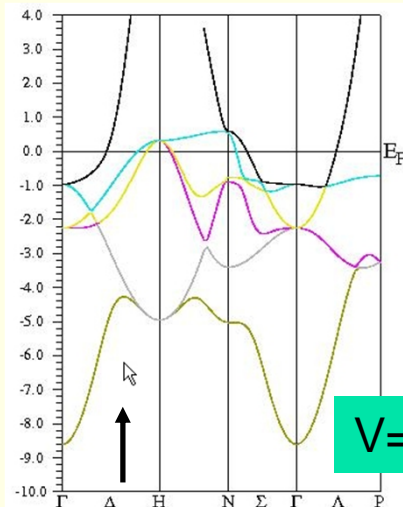Fe_vol___3.0_rk8_5000k.scf::MMTOT: 2.258
Fe_vol__-3.0_rk8_5000k.scf::MMTOT: 2.159
Fe_vol___6.0_rk8_5000k.scf::MMTOT: 2.320
Fe_vol__-6.0_rk8_5000k.scf::MMTOT: 2.114

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

V=-6%

V=+6%

- **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)*
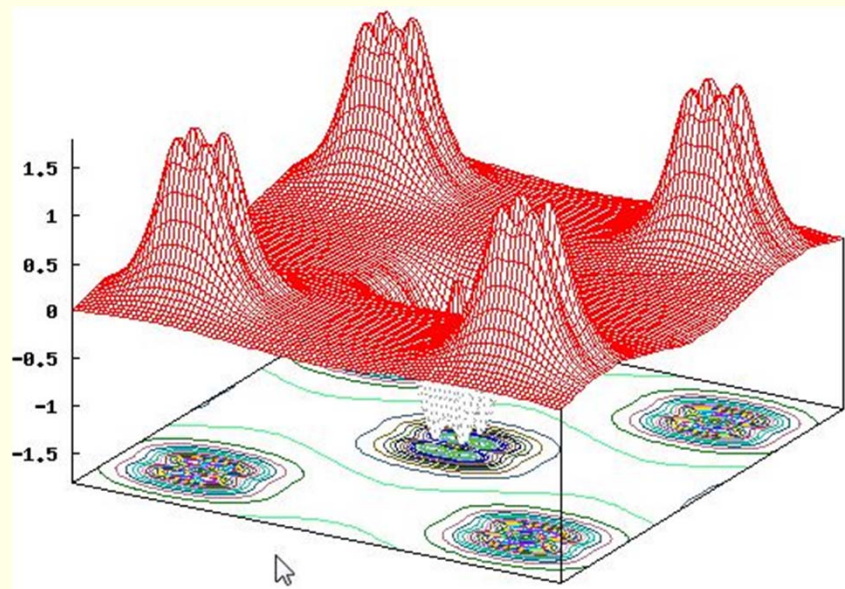
Exercise 6:

- **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)

  - *try a TB-mBJ calculation for NiO (start new case, starting from GGA; follow instructions given in P.Blaha's lecture) and compare gap/DOS*
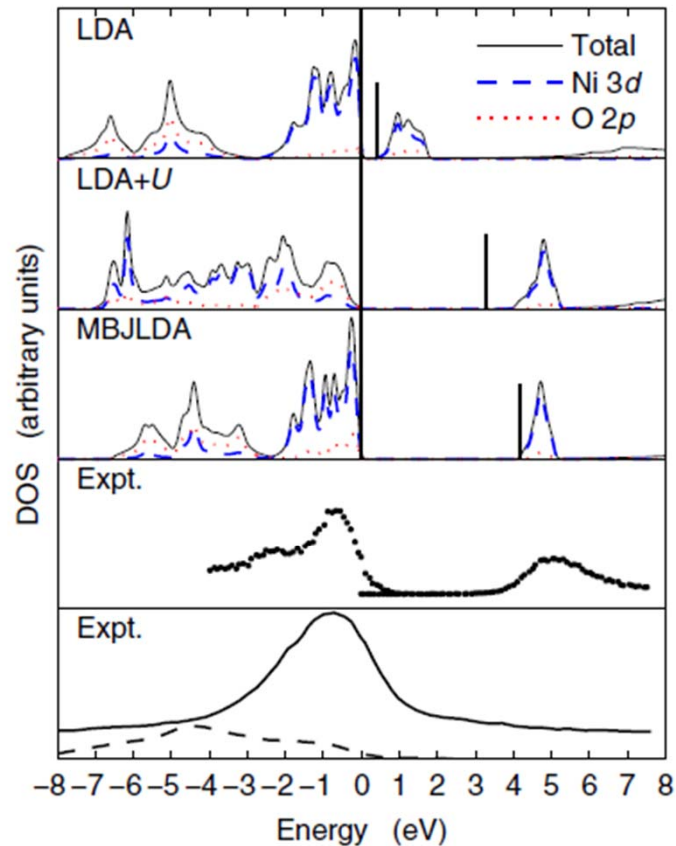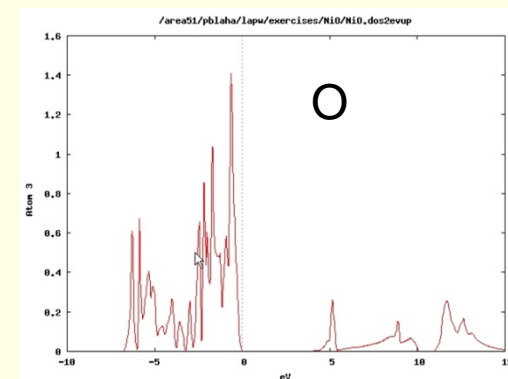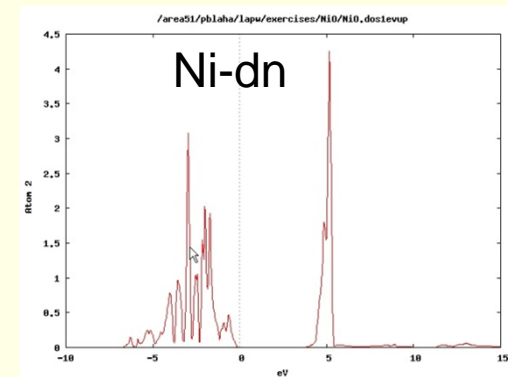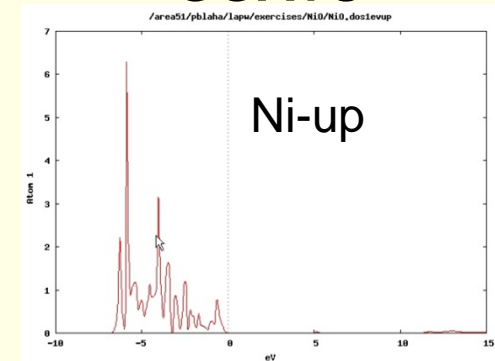
NiO cont…

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

Ni-up

Ni-dn

O

- ## 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 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
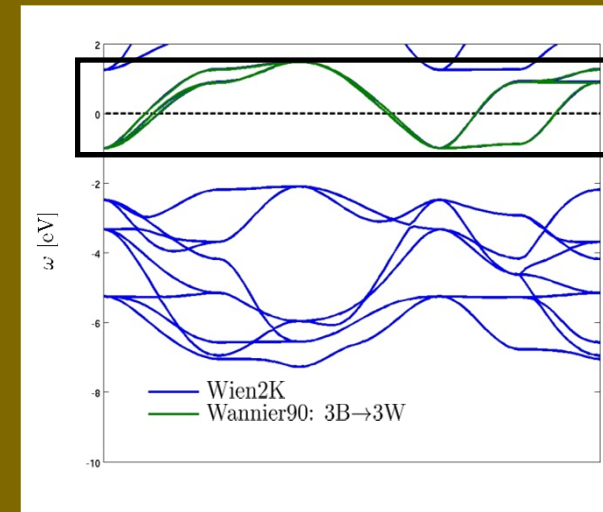
wien2wannier-exercise

- step by step

1) standard wien2k run, obtain bandstructure

2) identify target bands (choose low energy model)

3) identify character of bands (e.g. partial DOS)

4) init_w2w

5) x lapw1

6) w2w case

7) shift_energy case

8) wannier90.x case

9) consistency check (bands, spread)

1) standard wien2k run, obtain bandstructure
  - create SrVO3 struct; SG:221_Pm-3m;a=7.2613 bohr; Sr at (0,0,0) V at (1/2,1/2,1/2), O at (0,1/2,1/2)
  - init_lapw, run_lapw, obtain bandstructure and character plot

2) identify target bands (choose low energy model)
  - target model: 3 V-t2g bands around E_F
  - investigate bandstructure, find E_{min},E_{max} (in eV) that define your low energy model

3) identify character of bands
  - character is V-t2g in perfect octahedral environment
  - find V index (Vidx) in SrVO3.struct

4) init_w2w
  - choose small k-mesh (e.g. 4x4x4)
  - in write_w2win use <Vidx> d as character

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5) x lapw1; x lapw2 -fermi

6) w2w SrVO3

7) shift_energy SrVO3

8) wannier90.x SrVO3

9) consistency check (bands, spread)

- in SrVO3.wout look for "Final spread" (should be ~ 1.6 Å^2)

- in gnuplot: p "SrVO3.spaghetti_ene" u 4:5,
    "SrVO3_band.dat" u ($1*0.53):2 w l

10) beyond (ask P.Wissgott)

- plot Wannier orbitals, compute optical conductivity (woptic)