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)
- **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)*
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)
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 ΔV=1%.
- Another XC-potential (eg. PBEsol) will drastically change a₀.

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

![Graphs showing energy vs. volume for different RKmax values](attachment:image.png)
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), $a=b=3.15$ Å $c=4.77$ Å $\gamma=120^\circ$; 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)
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 `init_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
- xcrystalden --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
- xcrystalden --wien_struct 001.struct
- xcrystalden --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?**
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=makeupstructure(ac, [1 1 0], 1, 20., 30.);`
  - `showstruct(sr)`  # check out the number of layers and repeat the `sr=makeupstructure` 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 &`
- `xsgroup` 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 \((a_0=2.86 \text{ Å})\)
  - 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)

\[ V=-6\% \]
\[ V=+6\% \]
Exercise 6: antiferromagnetic calc.

- **Antiferromagnetism: bcc Cr \(a_0=2.885 \text{ Å}\) (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 "analysis"),
    - 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)
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
- xcrysdem --wien_struct NiO.struct  
  # visualize and understand the structure  
  # switch conventional/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: 1.41 μB)
  - compare orbital moments for SO and SO+U calculations (0.12 and 0.09 μB)
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)
Exercise 10: optical properties

- **Optical properties: fcc Al**
  - \(a_0=4.05\ \text{Å}\)
  - \textit{init\_lapw} (use 165 IBZ k-points only!)
  - \textit{run\_lapw}
  - \textit{calculate optics} (as described in the optics lecture, compare with the Al - Fig.)
    - calculate plasma frequency (\textit{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 \(a_0=4.08\ \text{Å}\))
  - \textit{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: \textit{run\_lapw} -so (case.inso \textbf{without RLOs} since optic does not support RLOs; put large Emax in case.in1); optics
Ag and Au: a relativistic effect

DOS

absorption

VISIBLE SPECTRUM
Exercise 11: Phonons of SrTiO₃

- This exercise should be done WITHOUT w2web in a terminal window!
- mkdir SrTiO3; cd SrTiO3;
- makestruct
  - SrTiO₃: 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
- your result should be like:
  phonons are unstable because SrTiO₃ has distorted, tetragonal structure at low temperatures
Exercise 12: Ga-NMR in BaGa₄

- This exercise should be done WITHOUT w2web in a terminal window!
- `mkdir BaGa4; cd BaGa4`
- `makestruct` (and type in the following information)
  - `BaGa₄`: 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 $\sigma_{iso}$ of both Ga atoms
  - `grep :EFG002 *scf`
  - `grep :EFG003 *scf`

- * 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 $c=HFF*1000$ (for a 100T field)
- 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; $\sigma_{sd}=(tot_{up}-tot_{dn})*10000$

<table>
<thead>
<tr>
<th>case</th>
<th>$V_{zz}(exp)$</th>
<th>$V_{zz}(th)$</th>
<th>$\delta_{iso}(exp)$</th>
<th>$\delta_{iso}(th)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ga1</td>
<td>5.99</td>
<td>3010</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ga2</td>
<td>1.20</td>
<td>840</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- $\sigma_{iso}(th)=\sigma_{orb}-\sigma_{c}-\sigma_{sd}$
- 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).