Wien2k tutorials

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Today, I will talk about :

- Structure and how to run the wien2k code
- Research strategies using first principle code
- Results of wien2k for two examples MnO and FeSe

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- **Structure and how to run the wien2k code**
- Research strategies
- Results of wien2k for two examples MnO and FeSe

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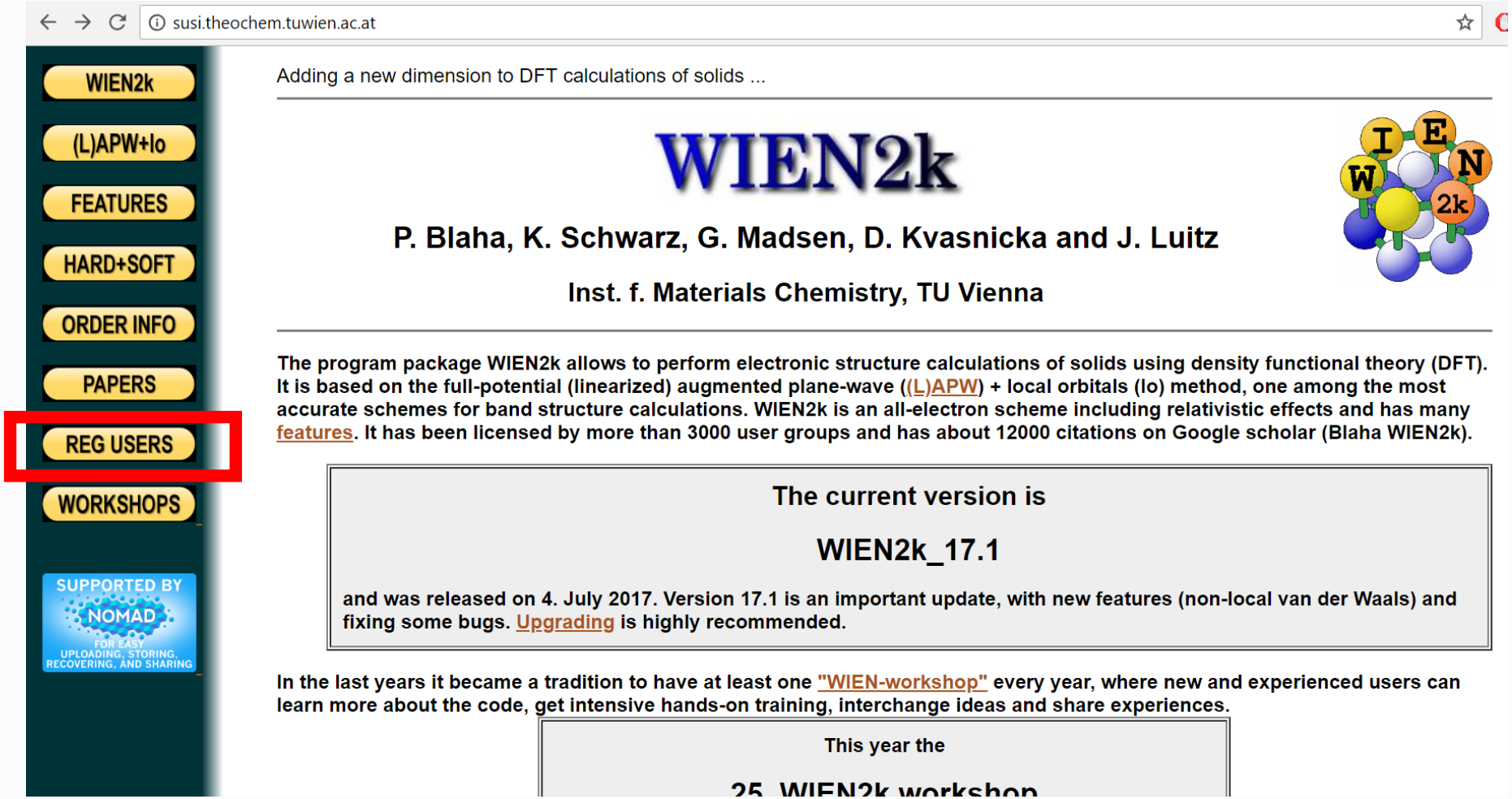
Structure and how to run the wien2k code :



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Structure and how to run the wien2k code :

susi.theochem.tuwien.ac.at/reg_user/textbooks/

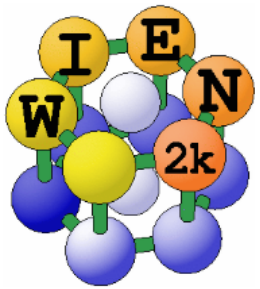
WIEN2k
(L)APW+lo
FEATURES
HARD+SOFT
ORDER INFO
PAPERS
REG USERS

Adding a new dimension to DFT calculations of solids ...

WIEN2k-Textbooks:

On this page you find links to usefull texts related to WIEN2k.

Please let us know it you have some interesting material which should be added to this list.



- Most recent version of the WIEN2k-Usersguide (pdf)
- DFT and the Family of (L)APW-methods: a step-by-step introduction (pdf)

A very nice introduction to DFT, (L)APW and the WIEN2k code by S.Cottenier (Univ. Gent, Belgium). Highly recommended for newcomers in this field. Updated Aug. 2013. (The old version is available from here.)

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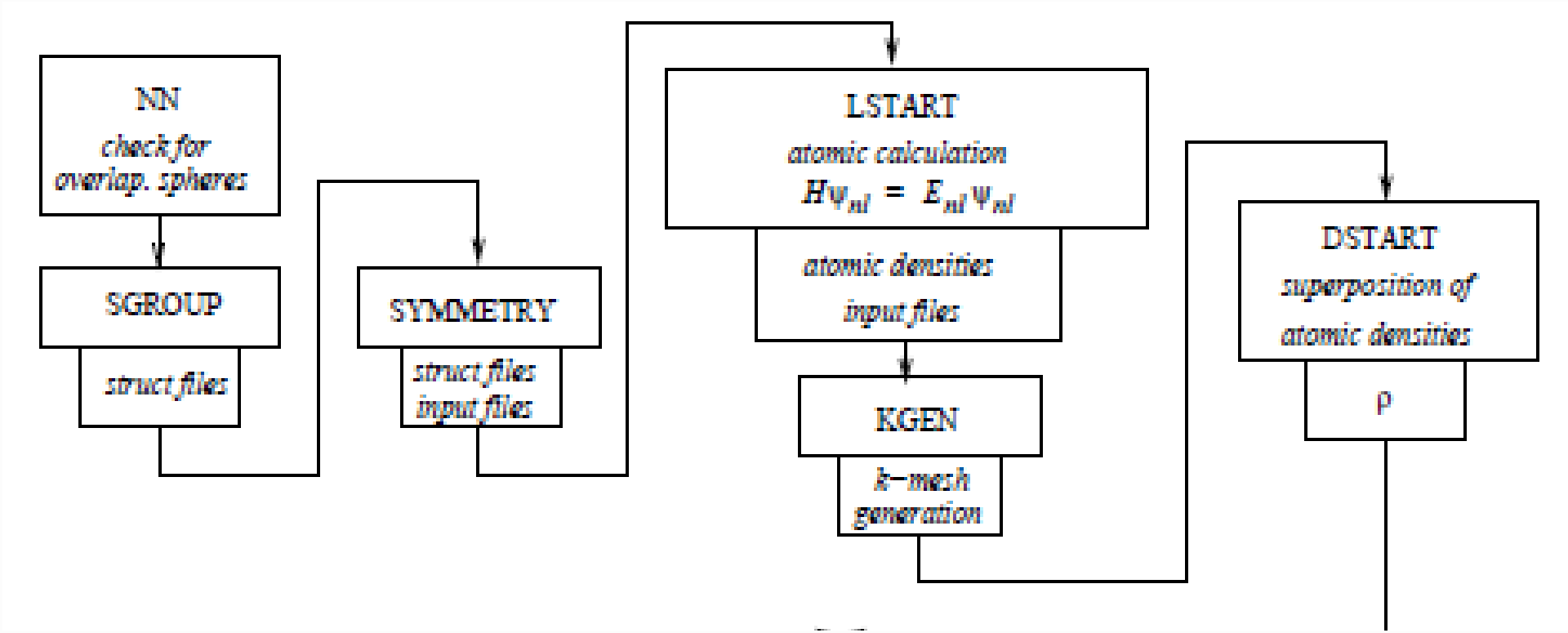
Structure and how to run the wien2k code :

- The code is very well structured in independent programs linked through scripts
- All we need to start a calculations is the **crystal structure of a material**

Structure and how to run the wien2k code :

- Initialization of a calculation … start from case.struct and run the script init_lapw



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Structure and how to run the wien2k code :

- Information on any program

```
init_lapw -h

PROGRAM: /zeus/WIEN2k/init_lapw
PURPOSE: initialisation of the l/apw-package WIEN2k
to be called within the case-directory
has to be located in WIEN-executable directory
needs case.struct  file
USAGE: init_lapw [OPTIONS] [FLAGS]
FLAGS:
-h/-H  ->help
-b ->batch (non-interactive) mode (see possible options below, SGROUP is always ignored)
-sp ->in batch mode: select spin-polarized calculation
OPTIONS:
-red X     ->in batch mode: RMT reduction by X % (default: RMT not changed)
-vxc X     ->in batch mode: VXC option (default: 13 = PBE )
-ecut X    ->in batch mode: energy seperation between core/valence (default: -6.0 Ry)
-rkmax X   ->in batch mode: RKMAX  (default: 7.0, not changed)
```

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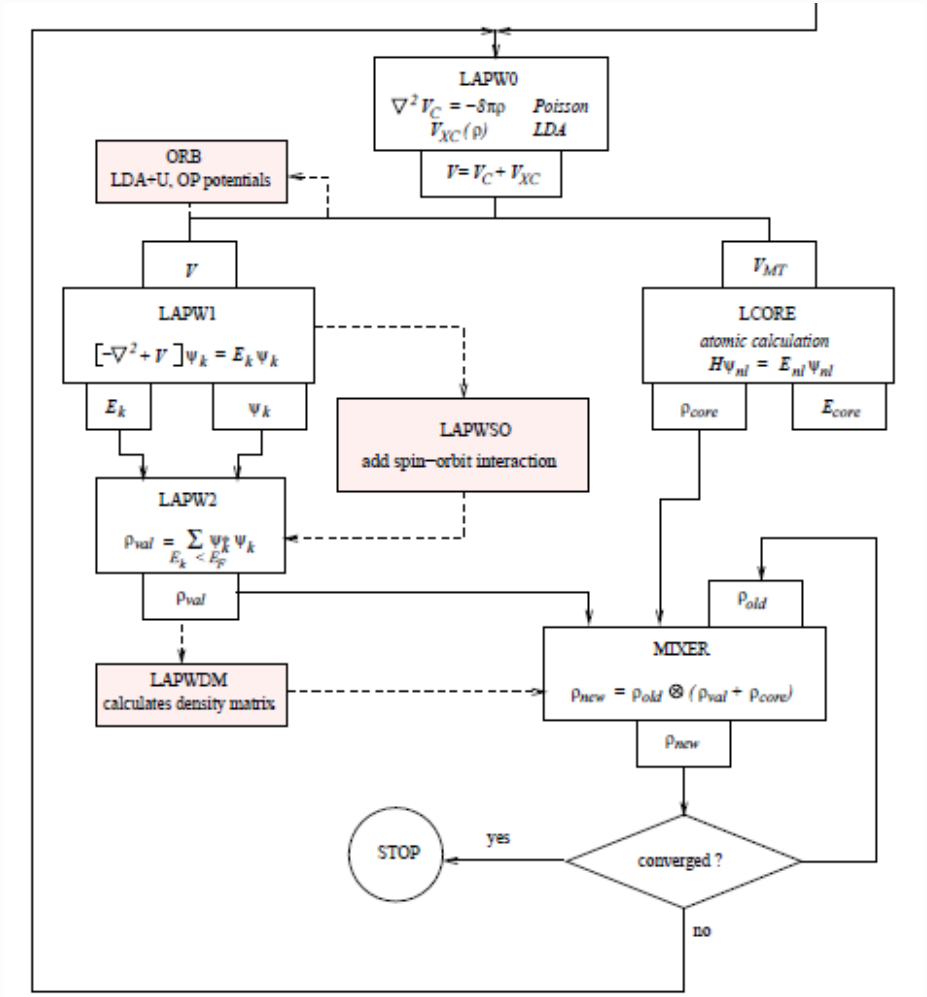
Structure and how to run the wien2k code :

- Program flow in wien2k
- To run a NON-MAGNETIC calculation run
- the script run_lapw

LAPW0 (POTENTIAL) generates potential from density
LAPW1 (BANDS) calculates valence bands (eigenvalues and eigenvectors)
LAPW2 (RHO) computes valence densities from eigenvectors
LCORE computes core states and densities
MIXER mixes input and output densities



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Structure and how to run the wien2k code :

- when if the calculation converged

```
run_lapw -h

PROGRAM:        /zeus/lapw/WIEN2k/bin/run_lapw

PURPOSE:        running the nonmagnetic scf-cycle in WIEN
                to be called within the case-subdirectory
                has to be located in WIEN-executable directory

USAGE:          run_lapw [OPTIONS] [FLAGS]

OPTIONS:
-cc LIMIT ->    charge convergence LIMIT (0.0001 e)
-ec LIMIT ->    energy convergence LIMIT (0.0001 Ry)
-fc LIMIT ->    force  convergence LIMIT (1.0 mRy/a.u.)
                default is -ec 0.0001; multiple convergence tests possible
```

Structure and how to run the wien2k code :

- Programs in wien2k

```
PURPOSE:runs WIEN executables:  afminput,aim,arrows,broadening,cif2struct,
      clmaddsub,clmcopy,clminter,convham,conv2prim,dftd3,dipan,dmftproj,
      dstart,eosfit,eosfit6,filtvec,findbands,fleur2wien,hex2rhomb,hf,
      initxspec,irrep,joint,joinvec,kgen,kram,lapw0,lapw1,lapw2,
      lapw3,lapw5,lapw7,lapwdm,lapwso,lcore,lorentz,lstart,mini,mixer,nn,
      optimize,orb,pairhess,plane,rhomb_in5,sgroup,shifteig,spaghetti,
      struct2cif,struct2poscar,struct_afm_check,sumpara,supercell,symmetry,
      symmetso,telnes3,tetra,txspec,wannier90,w2w,w2waddsp,wplot,xspec
```

Structure and how to run the wien2k code :

- Programs in wien2k

The "history" file case.scf

case.dayfile

:ENE	total energy (Ry). If there is a "WARNING" mentioned, check :WAR
:WAR	contains some warnings indicating that there might be a problem with your calculations. Usually these problems are not fatal, but may influence the accuracy.
:DIS	charge distance between last 2 iterations ($\int \|\rho_n - \rho_{n-1}\| dr$). Good convergence criterium.
:FER	Fermi energy (and Fermi-method)
:GAP	energy gap (for insulators). Please note, this value will only be correct, if the VBM/CBM are in your k-mesh. ("Shifted" k-meshes do not contain tha Gamma-point and often gaps are at Gamma !!)
:FORxx	force on atom xx in mRy/bohr (in the local (for each atom) cartesian coordinate system)
:FGLxx	force on atom xx in mRy/bohr (in the global coordinate system of the unit cell (in the same way as the atomic positions are specified))

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Research strategies using first principle code :

- Experimental crystal structure
- Crystallographic Information File (cif)

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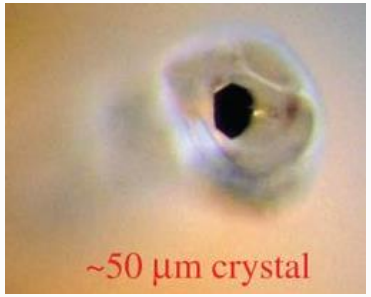
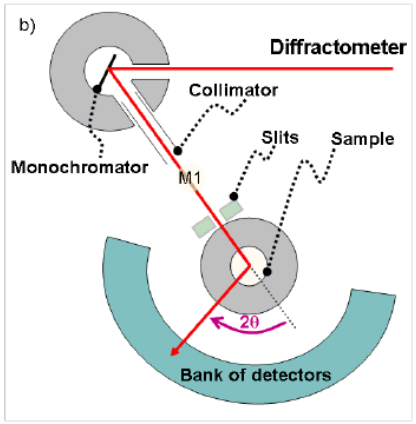
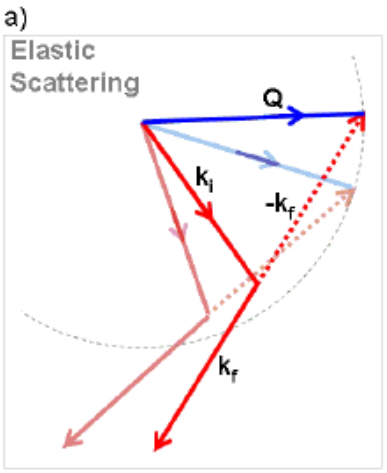
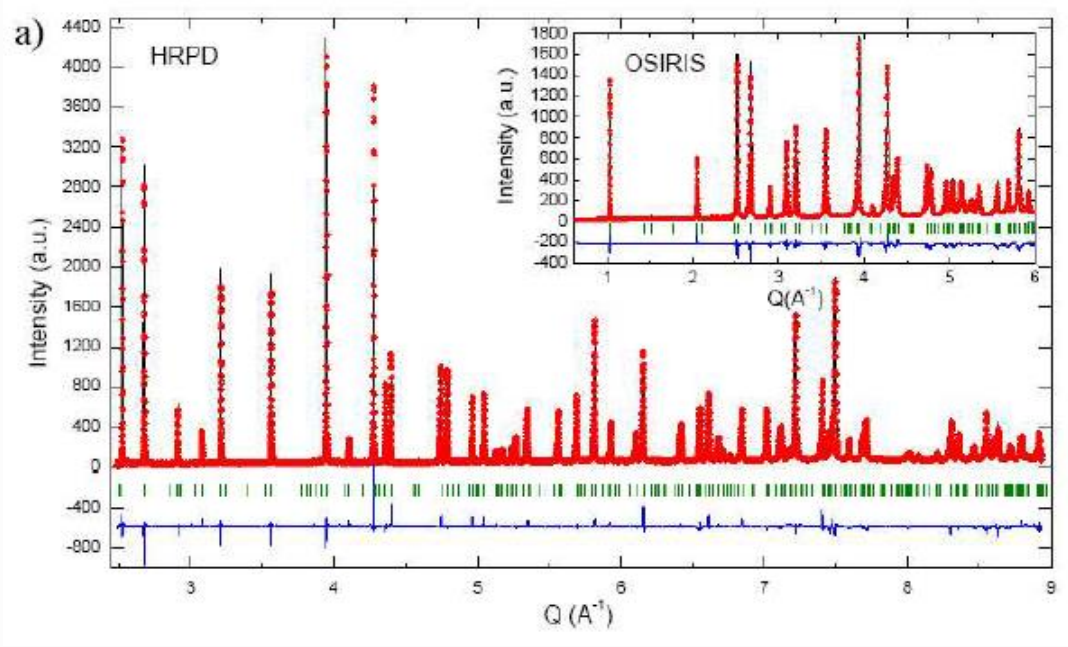
• Experimental crystal structure

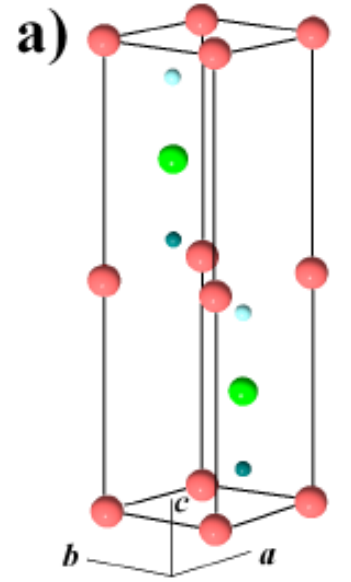






$P6_3/mmc$ (no. 194)		
$a_0 = 2.93919(5)$ Å		
$c = 12.2498(1)$ Å		
Atom	Site	(x, y, z)
Ni	$2a$	$(0, 0, 0)$
Ag	$2c$	$(\frac{2}{3}, \frac{1}{3}, \frac{1}{4})$
O	$4f$	$(\frac{2}{3}, \frac{1}{3}, z_O)$





Crystallographic Information File (cif)

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- Crystallographic

  Information File (cif)

- cif2struct MnO.cif
- MnO.struct

MnO.cif

```
# CRYSTAL DATA

#------------------------------------------------------------------------------

_chemical_name_common                  'MnO'
_cell_length_a                         4.44570
_cell_length_b                         4.44570
_cell_length_c                         4.44570
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      90
_symmetry_space_group_name_H-M         'F m -3 m'
_symmetry_Int_Tables_number            225

loop_
_space_group_symop_operation_xyz
   'x, y, z'
   '-x, -y, -z'
   ...
   'z+1/2, y+1/2, x'

loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
   Mn         1.0     0.000000      0.000000      0.000000     Biso  1.000000 Mn
   O          1.0     0.500000      0.500000      0.500000     Biso  1.000000 O
```

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Let’s start with the case

MnO (insulator)

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First, let's start a calculation on MnO – structural file :

- srun --mem 8GB -c 1 -t 1:00:00 --pty bash
- module load edmftf
- mkdir MnO - create a work directory for this project
- cd MnO - go inside that directory

```
@cp1434-mp2 ~]$ mkdir MnO
@cp1434-mp2 ~]$ cd MnO
@cp1434-mp2 MnO]$
```

- **cp $RESULTS/DFT/MnO.cif .** - copy the file containing the structure

First, let's start a calculation on MnO – structural file :

- cif2struct MnO.cif - convert the structural information to the wien2k format
- ls -l - check that a new file MnO.struct was created

```
[lect10@cp1434-mp2 MnO]$ ls
MnO.cif
[lect10@cp1434-mp2 MnO]$ cif2struct MnO.cif
[lect10@cp1434-mp2 MnO]$ ls -l
total 5
-rw-r--r-- 1 lect10 lect 4920 Jun  3 20:39 MnO.cif
-rw-r--r-- 1 lect10 lect  865 Jun  3 20:40 MnO.struct
[lect10@cp1434-mp2 MnO]$
```

First, let's start a calculation on MnO – structural file :

- less MnO.struct - see the contained of the file and press q to close the view

```
blebleble
F   LATTICE,NONEQUIV.ATOMS   2  225 Fm-3m
MODE OF CALC=RELA unit=bohr
  8.401155  8.401155  8.401155 90.000000 90.000000 90.000000
ATOM  -1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT=15
Mn         NPT=  781  R0=.000050000 RMT=   2.00000   Z:  25.00000
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT=15
O          NPT=  781  R0=.000100000 RMT=   2.00000   Z:   8.00000
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
   0      NUMBER OF SYMMETRY OPERATIONS
(END)
```

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First, let's start a calculation on MnO – prepare the job:

- init_lapw -b -vxc 5 -ecut -6.0 -rkmax 7 -numk 3000 - initialize the calculation

```
init_lapw -h

PROGRAM: /zeus/WIEN2k/init_lapw
PURPOSE: initialisation of the l/apw-package WIEN2k
to be called within the case-directory
has to be located in WIEN-executable directory
needs case.struct  file
USAGE: init_lapw [OPTIONS] [FLAGS]
FLAGS:
-h/-H  ->help
-b ->batch (non-interactive) mode (see possible options below, SGROUP is always ignored)
-sp ->in batch mode: select spin-polarized calculation
OPTIONS:
-red X     ->in batch mode: RMT reduction by X % (default: RMT not changed)
-vxc X     ->in batch mode: VXC option (default: 13 = PBE )
-ecut X    ->in batch mode: energy seperation between core/valence (default: -6.0 Ry)
-rkmax X   ->in batch mode: RKMAX  (default: 7.0, not changed)
-numk X    ->in batch mode: use X k-points in full BZ (default: 1000)
```

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First, let's start a calculation on MnO – structural file :

- ls - see the new files

```
[lect10@cp1434-mp2 MnO]$ ls
dstart.def    MnO.in0      MnO.inc             MnO.klist         MnO.rsigma        MnO.struct_st
dstart.error  MnO.in0_st   MnO.inc_st          MnO.nnshells      MnO.rsp           MnO.test
kgen.def      MnO.in0_std  MnO.inm             MnO.outputd       MnO.rspdn         MnO.tmp
:log          MnO.in1      MnO.inm_restart_st  MnO.outputkgen    MnO.rspup         MnO.tmpden
lstart.def    MnO.in1_st   MnO.inm_st          MnO.outputnn      MnO.sigma         MnO.vspdn_st
MnO.bva       MnO.in2      MnO.inq             MnO.outputs       MnO.struct        MnO.vsp_st
MnO.cif       MnO.in2_ls   MnO.inq_st          MnO.outputsgroup  MnO.struct_nn     new_super.clmsum
MnO.clmsum    MnO.in2_st   MnO.inst            MnO.outputsgroup1 MnO.struct_orig   nn.def
MnO.dayfile   MnO.in2_sy   MnO.kgen            MnO.outputst      MnO.struct_sgroup symmetry.def
[lect10@cp1434-mp2 MnO]$
```

First, let's start a calculation on MnO – prepare the job:

- run_lapw -ec 0.0001 -cc 0.0001 - run the calculation

```
      run_lapw -h


PROGRAM:        /zeus/lapw/WIEN2k/bin/run_lapw

PURPOSE:        running the nonmagnetic scf-cycle in WIEN
                to be called within the case-subdirectory
                has to be located in WIEN-executable directory

USAGE:          run_lapw [OPTIONS] [FLAGS]

OPTIONS:
-cc LIMIT ->    charge convergence LIMIT (0.0001 e)
-ec LIMIT ->    energy convergence LIMIT (0.0001 Ry)
-fc LIMIT ->    force  convergence LIMIT (1.0 mRy/a.u.)
                default is -ec 0.0001; multiple convergence tests possible
```

Today, I will talk about :

- Structure and how to run the wien2k code
- **Research strategies using first principle code**
- Results of wien2k

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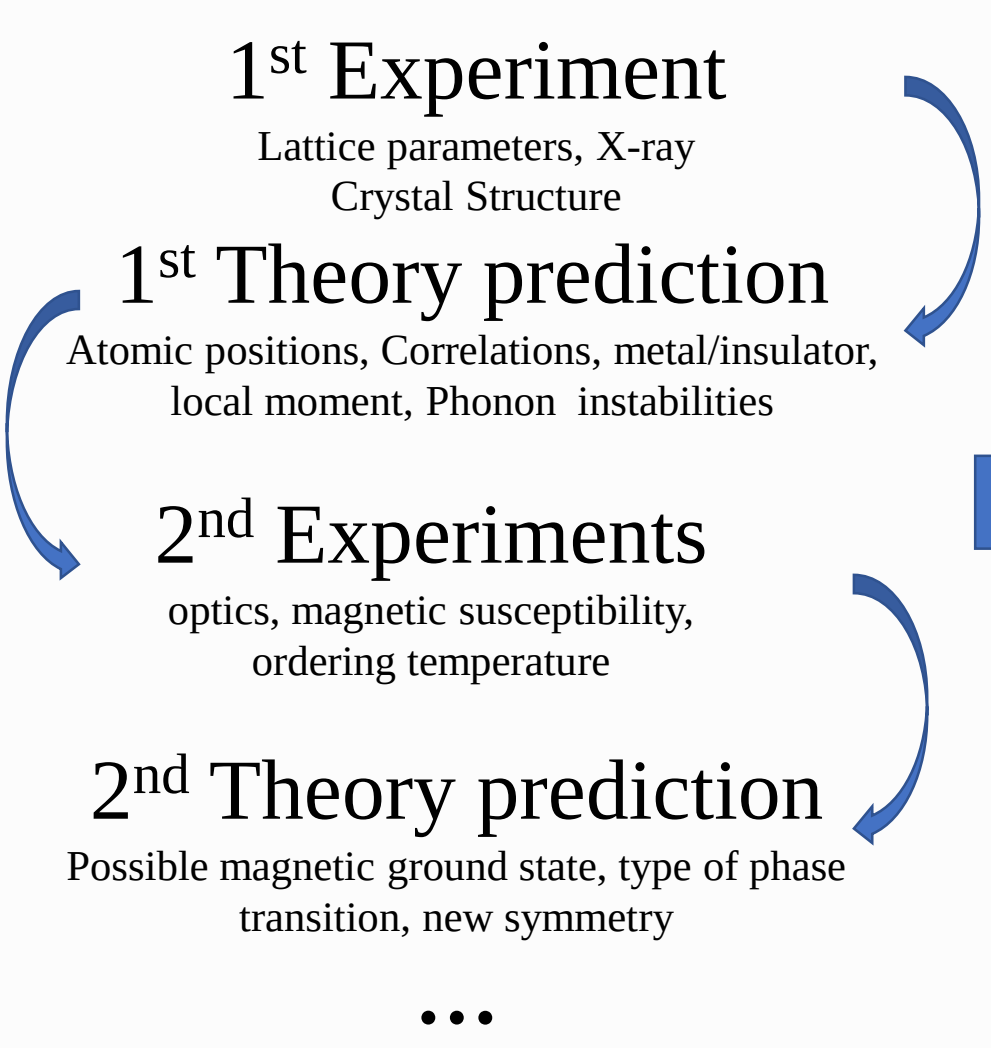

Self-consistent experiment + theory?

- novel states of matter
- new functionalities
- improve existing materials/functionalities

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Before I will give example for the research strategy

Let's continue with another calculation

FeSe (metal)

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Now, let's start a calculation on FeSe – structural file :

- We are inside the MnO directory -
- cp ../ - let's go outside

```
[lect10@cp1434-mp2 MnO]$ cd ../
[lect10@cp1434-mp2 ~]$ mkdir FeSe
[lect10@cp1434-mp2 ~]$ cd FeSe
[lect10@cp1434-mp2 FeSe]$
```

- mkdir FeSe - create a work directory for this project
- cd FeSe - go inside the new directory
- cp **$RESULTS/DFT/**FeSe.struct . - copy the file containing the structure

Now, let's start a calculation on FeSe – structural file :

- less FeSe.struct - see the contained of the file and press q to close the view

```
FeSe structure
P                           2  129 P4/nmm
             RELA
  7.121433  7.121433 10.430154 90.000000 90.000000 90.000000
ATOM  -1: X=0.25000000 Y=0.75000000 Z=0.00000000
          MULT= 2           ISPLIT=-2
      -1: X=0.75000000 Y=0.25000000 Z=0.00000000
Fe  2+     NPT=  781  R0=0.00005000 RMT= 2.31        Z:  26.00000
LOCAL ROT MATRIX:    0.7071068-0.7071068 0.0000000
                     0.7071068 0.7071068 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.75000000 Y=0.75000000 Z=0.73000000
          MULT= 2           ISPLIT=-2
      -2: X=0.25000000 Y=0.25000000 Z=0.27000000
Se  2-     NPT=  781  R0=0.00005000 RMT= 2.20        Z:  34.00000
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  16       NUMBER OF SYMMETRY OPERATIONS
```

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Now, let's start a calculation on FeSe – prepare the job:

- init_lapw -b -vxc 5 -ecut -6.0 -rkmax 7 -numk 1000 - initialize the calculation
- ls - to check how many files were created
- run_lapw -ec 0.0001 -cc 0.0001 -fc 1 - run the calculation

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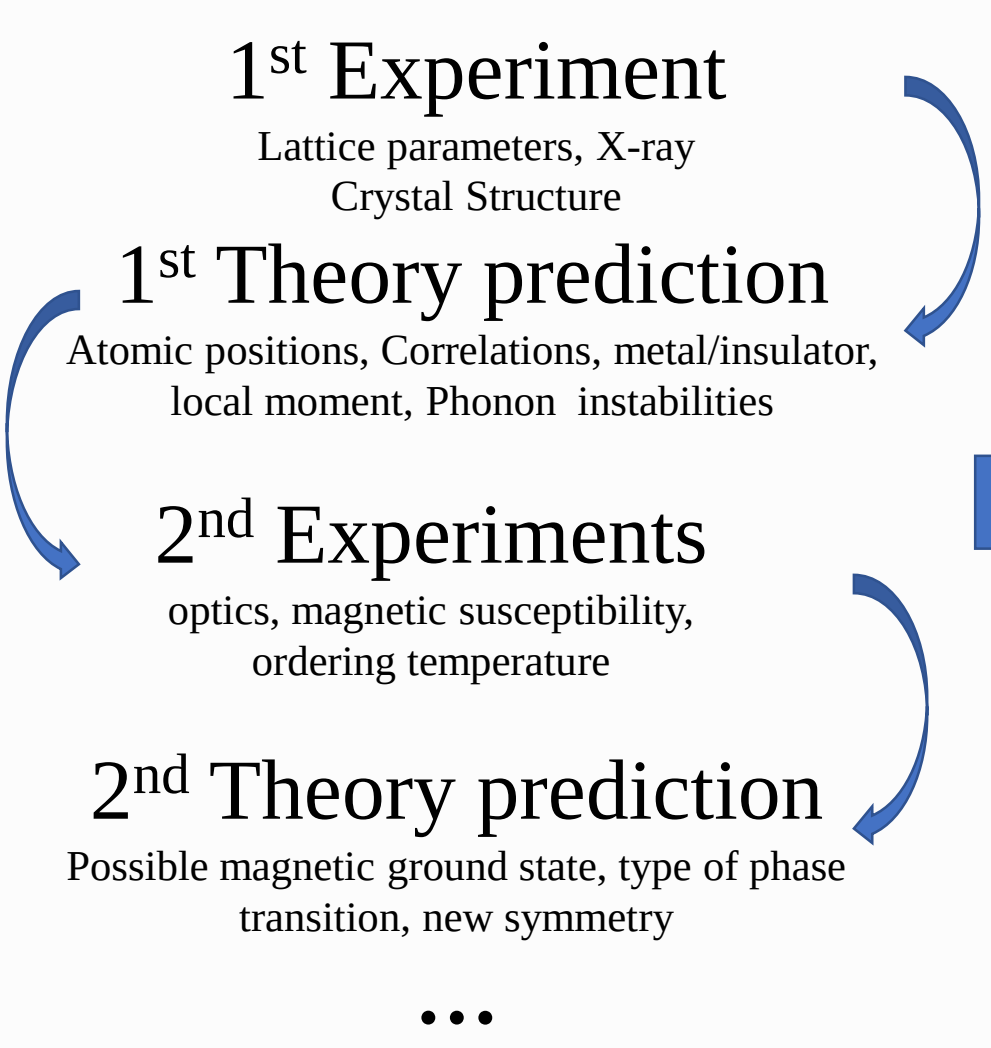

Self-consistent experiment + theory?

- novel states of matter
- new functionalities
- improve existing materials/functionalities

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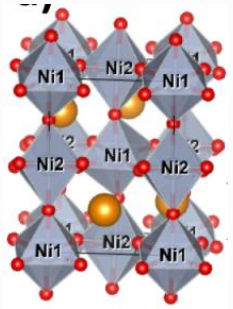
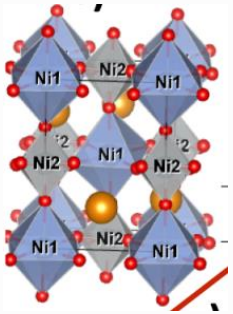
$ReNiO_3$

high temperature



low temperature



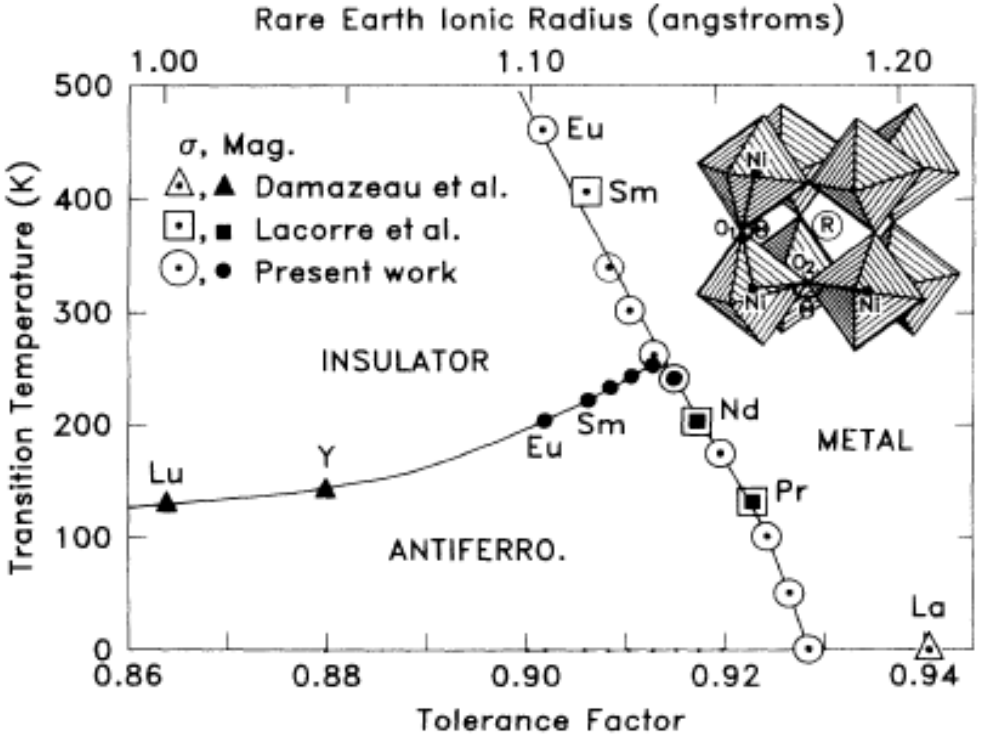


FIG. 2. Insulator-metal-antiferromagnetic phase diagram for RNiO$_3$ as a function of the tolerance factor and (equivalently) the ionic radius of the rare earth (R).

Phys. Rev. B **45**, 8209(R)

At low-T

"**charge disproportionation**" ???

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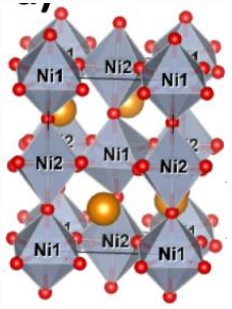
Forces in DFT+DMFT: Crystal/Magnetic Structure predictions



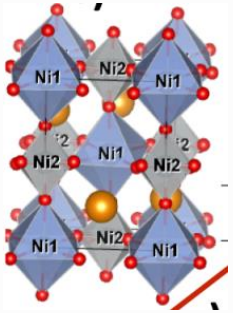


TABLE I: Optimized atomic positions in the metallic and insulating state of $NdNiO_3$. Experimental structure is from Ref. 8. The GGA and GGA+U structure is from Ref. 6.

Pbnm	Exp.	DMFT-PARA	GGA
Ni	(0.000, 0.000, 0.500)	(0.000, 0.000, 0.500)	(0.000, 0.000, 0.500)
O_1	(0.216, 0.287, 0.539)	(0.214, 0.287, 0.539)	(0.207, 0.294, 0.547)
O_2	(0.569, 0.490, 0.750)	(0.573, 0.490, 0.750)	(0.591, 0.477, 0.750)
Nd	(0.496, 0.035, 0.750)	(0.491, 0.044, 0.750)	(0.488, 0.058, 0.750)
$\sqrt{\langle(\mathbf{r}-\mathbf{r}_{exp})^2\rangle}$		0.0056	0.0190
$P2_1/n$	Exp	DMFT-AFM	GGA+U
Ni_1	(0.000, 0.000, 0.000)	(0.000, 0.000, 0.000)	(0.000, 0.000, 0.000)
Ni_2	(0.000, 0.000, 0.500)	(0.000, 0.000, 0.500)	(0.000, 0.000, 0.500)
O_1	(0.575, 0.487, 0.752)	(0.574, 0.489, 0.750)	(0.595, 0.475, 0.755)
O_2	(0.214, 0.276, 0.527)	(0.209, 0.285, 0.540)	(0.198, 0.291, 0.549)
O_3	(0.719, 0.204, 0.447)	(0.717, 0.210, 0.460)	(0.711, 0.198, 0.452)
Nd	(0.493, 0.039, 0.750)	(0.493, 0.044, 0.750)	(0.489, 0.056, 0.750)
$\sqrt{\langle(\mathbf{r}-\mathbf{r}_{exp})^2\rangle}$		0.0091	0.0180

Kristjan Haule and **Gheorghe L. Pascut**, Phys. Rev. B **94**, 195146 (2016)

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Wien2k tutorial

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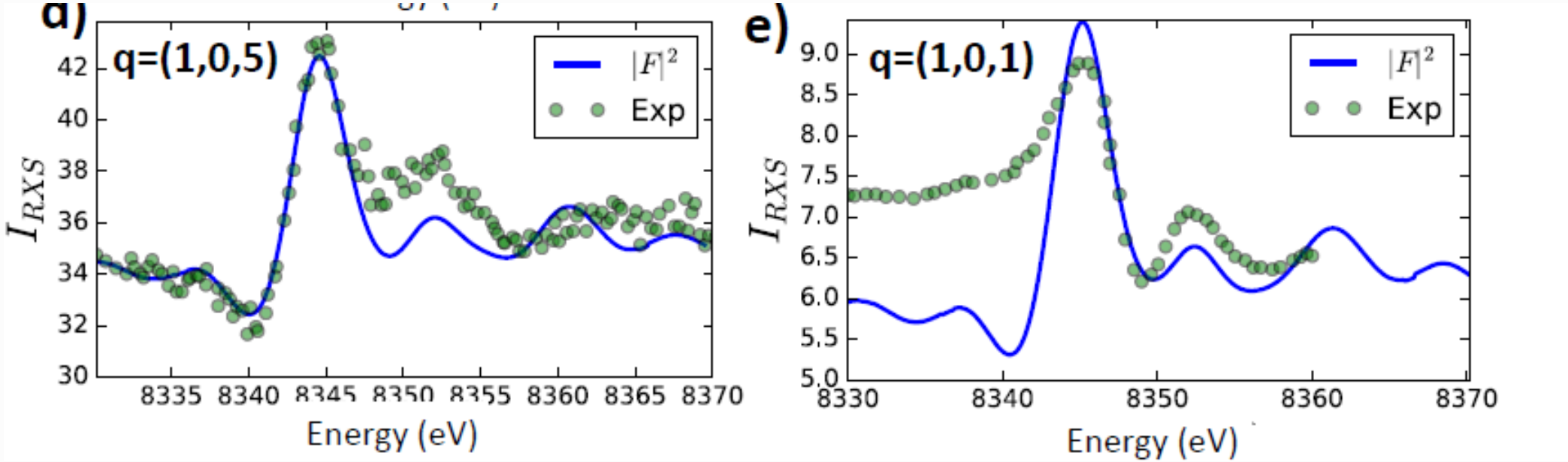
Resonant X-ray Scattering from DFT+DMFT



"**charge disproportionation**" ???

Kristjan Haule and **Gheorghe L. Pascut, Scientific Reports**

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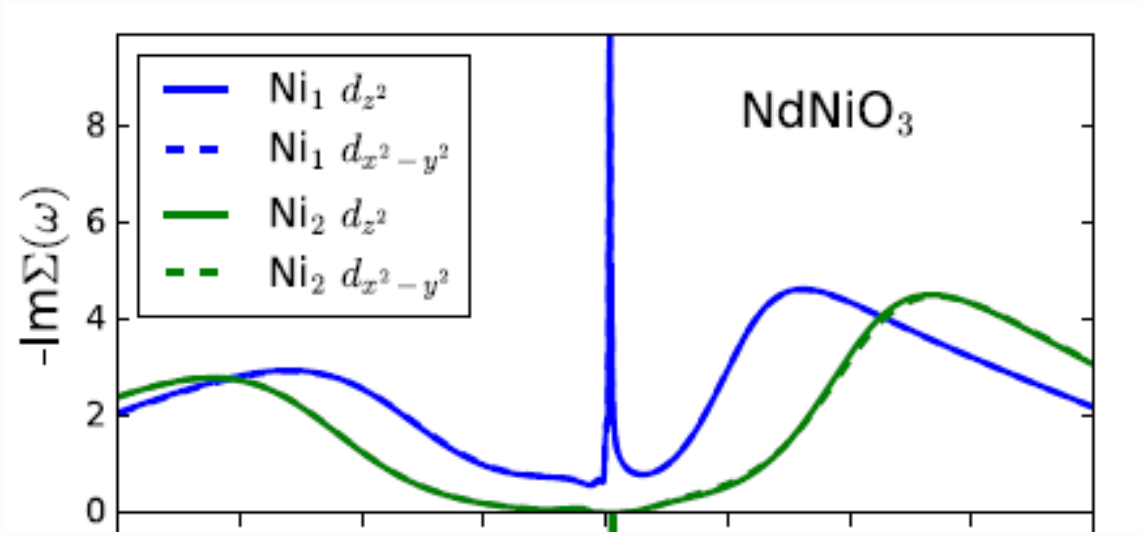
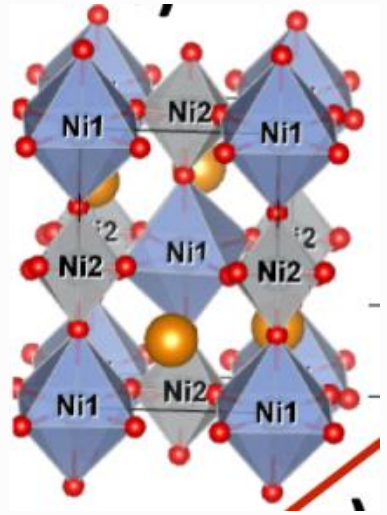
DFT+DMFT – magnetic predictions





DFT + DMFT – paramagnetic state

Half of the Ni ions have exactly zero magnetic moment!!!

Kristjan Haule and **Gheorghe L. Pascut, Scientific Reports**

*Gheorghe **Lucian** Pascut, Department of Physics & Astronomy , Rutgers The State University of New Jersey, USA (glucian.pascut@gmail.com)*

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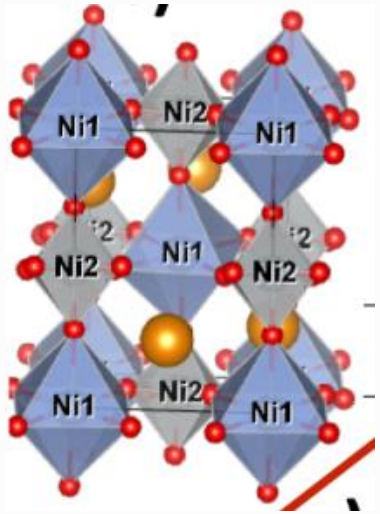
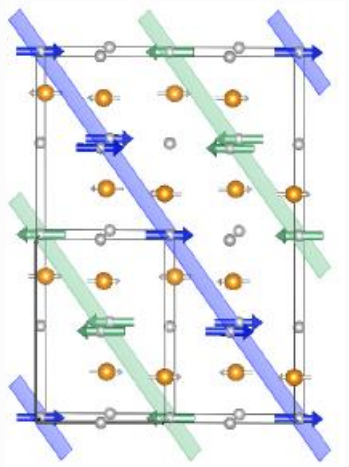
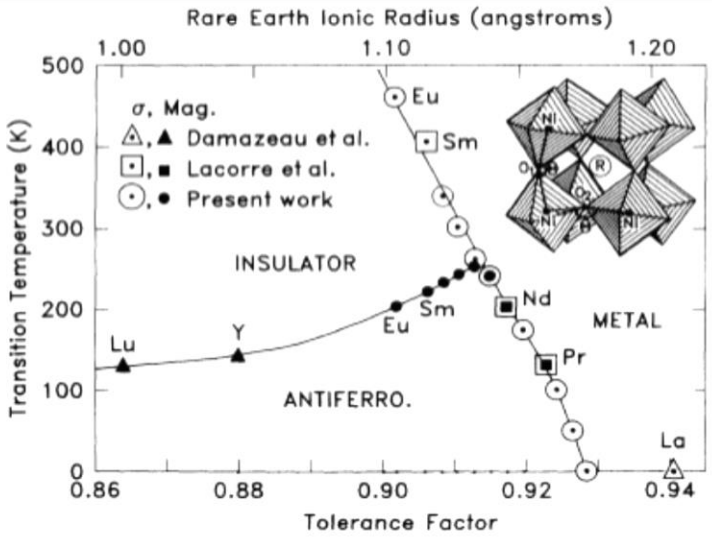
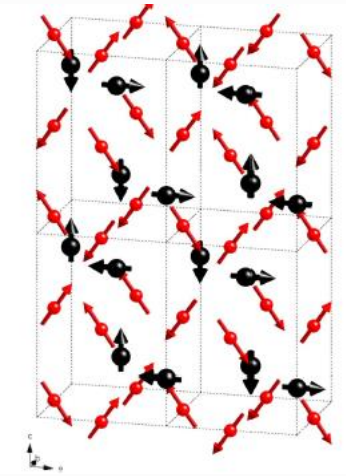
Proposed - $NdNiO_3$

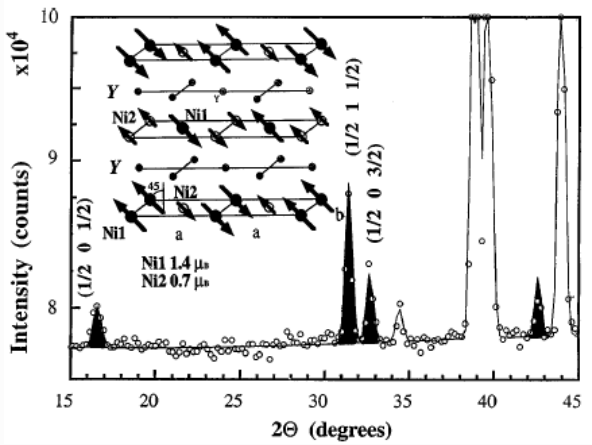




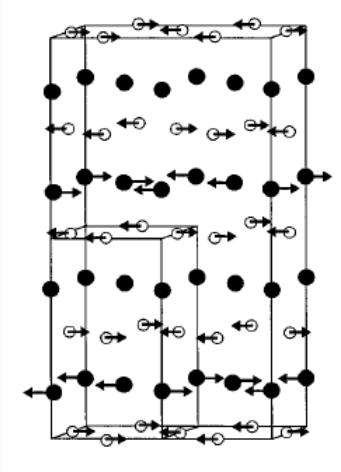




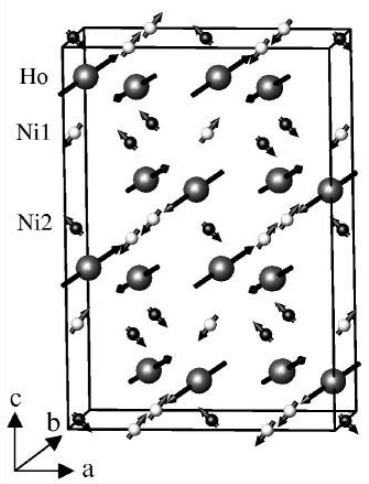
$YNiO_3$



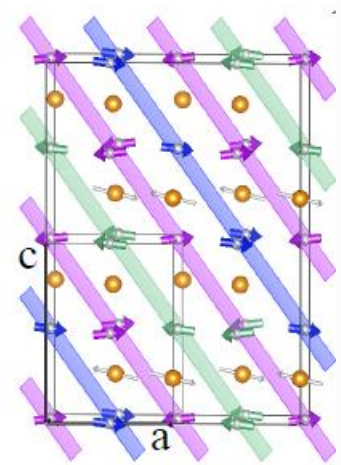
$(Sm,Eu)NiO_3$



$HoNiO_3$



$(Pr,Nd)NiO_3$



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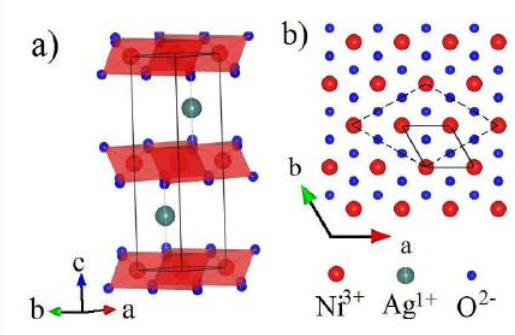
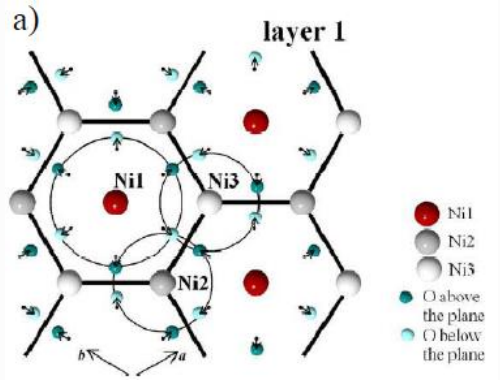
$AgNiO_2$

High-T



metal

Low-T



bad-metal

Gheorghe L. Pascut et. all
PRL 106, 157206 (2011)

$ReNiO_3$

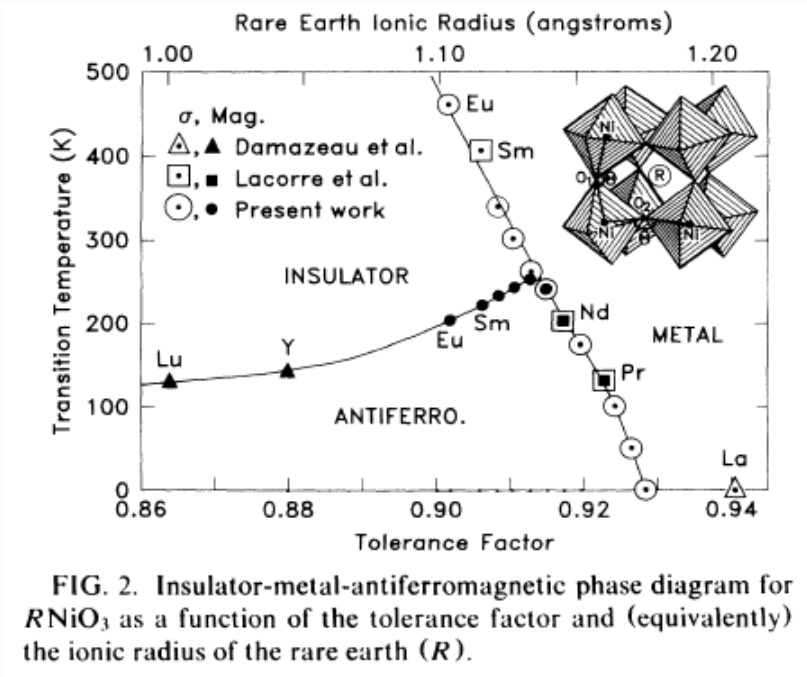
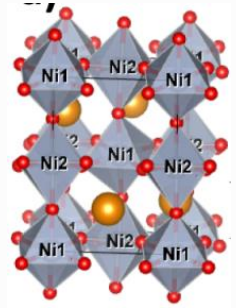


FIG. 2. Insulator-metal-antiferromagnetic phase diagram for $RNiO_3$ as a function of the tolerance factor and (equivalently) the ionic radius of the rare earth (R).

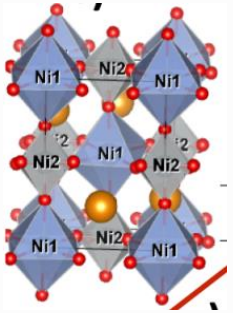
At low-T both compounds show
"charge disproportionation"

Phys. Rev. B **45**, 8209(R)

high temperature



low temperature



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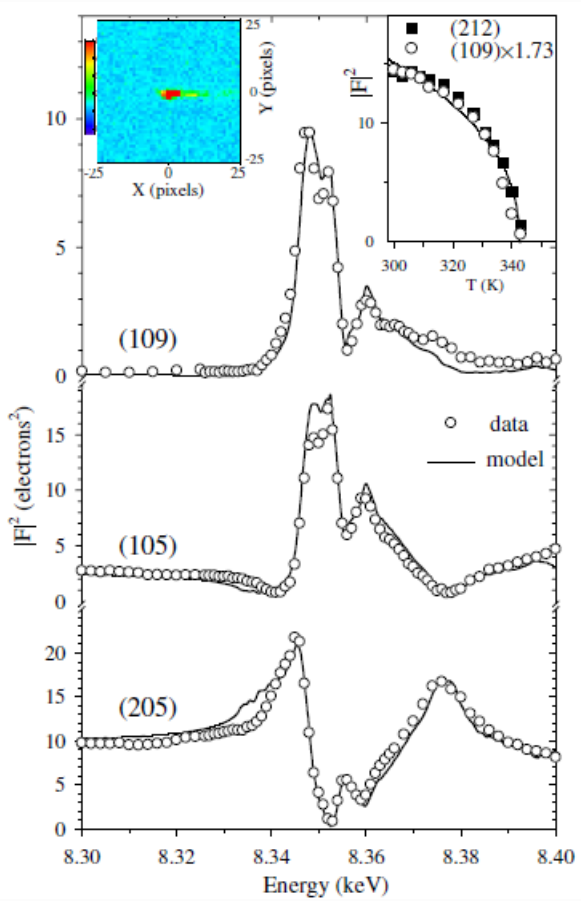
Resonant X-ray Scattering – $AgNiO_2$

Results accepted as evidence
for
charge disproportionation

DFT give a negligible charge disproportionation which is also depended on the details of the calculations



Gheorghe L. Pascut et. all PRL 106, 157206 (2011)

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What else can we do?

Structural relaxations in the paramagnetic state

Tricks in DFT don't work …

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Today, I will talk about :

- Structure and how to run the wien2k code
- Research strategies using first principle code
- Results of wien2k for two examples MnO and FeSe

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Results of wien2k for FeSe and MnO

- Density of states
- Band structure
- Band structure with band character plotting

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Results of wien2k for FeSe

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Wien2k tutorial

Results of wien2k for FeSe - You should be in the FeSe dir

- grep :CHA FeSe.dayfile - charge convergence

run_lapw -ec 0.0001 -cc 0.0001 -fc 1

```
[lect10@cp1434-mp2 FeSe]$ grep :CHA FeSe.dayfile
:CHARGE convergence:  0 0.0001 0
:CHARGE convergence:  0 0.0001 0
:CHARGE convergence:  0 0.0001 .2732603
:CHARGE convergence:  0 0.0001 .3751676
:CHARGE convergence:  0 0.0001 .1349825
:CHARGE convergence:  0 0.0001 .0974887
:CHARGE convergence:  0 0.0001 .0132406
:CHARGE convergence:  0 0.0001 .0074044
:CHARGE convergence:  0 0.0001 .0016225
:CHARGE convergence:  0 0.0001 .0004805
:CHARGE convergence:  0 0.0001 .0001906
:CHARGE convergence:  1 0.0001 -.0000576
:CHARGE convergence:  1 0.0001 -.0000685
[lect10@cp1434-mp2 FeSe]$
```

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Results of wien2k for FeSe - You should be in the FeSe dir

- grep :ENE FeSe.dayfile - energy convergence

run_lapw -ec 0.0001 -cc 0.0001 -fc 1

```
[lect10@cp1434-mp2 FeSe]$ grep :ENE FeSe.dayfile
:ENERGY convergence:  0 0.0001 0
:ENERGY convergence:  0 0.0001 0
:ENERGY convergence:  0 0.0001 .0220166350000000
:ENERGY convergence:  0 0.0001 .0300415950000000
:ENERGY convergence:  0 0.0001 .0213419950000000
:ENERGY convergence:  0 0.0001 .0094099950000000
:ENERGY convergence:  0 0.0001 .0031383150000000
:ENERGY convergence:  0 0.0001 .0006063200000000
:ENERGY convergence:  1 0.0001 .0000149650000000
:ENERGY convergence:  1 0.0001 .0000087750000000
:ENERGY convergence:  1 0.0001 .0000054050000000
:ENERGY convergence:  1 0.0001 .0000033000000000
:ENERGY convergence:  1 0.0001 .0000017500000000
[lect10@cp1434-mp2 FeSe]$
```

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Results of wien2k for FeSe - You should be in the FeSe dir

- grep :FOR FeSe.dayfile - energy convergence

run_lapw -ec 0.0001 -cc 0.0001 -fc 1

```
[lect10@cp1434-mp2 FeSe]$ grep :FOR FeSe.dayfile
:FORCE convergence: 1 1 0 XCO 0 XCO
```

Results of wien2k for FeSe - You should be in the FeSe dir

- mkdir FeSe
- cp * **FeSe**

SAVE the calculation for DMFT

Density of states

- x lapw1
- x lapw2 -qtl

```
[lect10@cp1433-mp2 FeSe]$  x lapw1
 LAPW1 END
76.630u 2.570s 0:40.12 197.4%   0+0k 0+154784io 0pf+0w
[lect10@cp1433-mp2 FeSe]$
```

```
[lect10@cp1433-mp2 FeSe]$ x lapw2 -qtl
 LAPW2 END
15.966u 1.333s 0:10.60 163.1%   0+0k 0+127080io 0pf+0w
[lect10@cp1433-mp2 FeSe]$
```

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Results of wien2k for FeSe - You should be in the FeSe dir

- **Density of states**
- configure_int_lapw
- 1
- tot,s,p,d,f
- 2
- tot,s,pd,f
- total
- end

```
[lect10@cp1433-mp2 FeSe]$ configure_int_lapw
     (C)2008 by Morteza Jamal
#################################
#                               #
 Configures and creates FeSe.int
#                               #
#################################

atom 1 is Fe
atom 2 is Se

*** For Total DOS type 'total' ***

*** For finishing type 'end' ***

Please enter the number of atom that you like to plot DOS? (default:1) 1
Select PDOS for Fe from: tot,s,p,pz,px+py,d,dz2,dxy,dx2y2,dxz+dyz,f (give a comma-separated list).
tot,s,p,d,f

*** For finishing type 'end' ***

Please enter the number of atom that you like to plot DOS? (default:2) 2
Select PDOS for Se from: tot,s,p,pz,px+py,d,dz2,dxy,dx2y2,dxz+dyz,f (give a comma-separated list).
tot,s,p,d,f

*** For finishing type 'end' ***

Please enter the number of atom that you like to plot DOS? (default:3) total

*** For finishing type 'end' ***

Please enter the number of atom that you like to plot DOS? (default:4) end

FeSe.int is ready for using.

[lect10@cp1433-mp2 FeSe]$
```

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Results of wien2k for FeSe - You should be in the FeSe dir

Density of states

- x tetra

```
[lect10@cp1433-mp2 FeSe]$ x tetra
 openfilename:
 FeSe.dos2


 LEGAL END TETRA
0.344u 0.015s 0:00.39 89.7%     0+0k 2440+1184io 1pf+0w
[lect10@cp1433-mp2 FeSe]$
```

- **Open a new terminal**
- **module load edmftf**
- dosplot2

```
     (C)2007 by Morteza Jamal
####################################
#                                  #
#            DOS PLOT 2            #
#                                  #
####################################

NOTE: This plotting interface uses FeSe.int and FeSe.qtl
      thus, these files must correspond to your FeSe.dos[1-7][ev] files.
      At present we support up to 49 DOS cases.


Which units?
     Ryd .. 0
     eV  .. 1 (default)
1
```

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Results of wien2k for FeSe - You should be in the FeSe dir

Density of states

- dosplot2

```
*ATTENTION*
You can select 11 + 0  DOS for plotting in FeSe.int .

Please see and select lines to plot.

 line:1 (tot) of atom Fe
 line:2 (s) of atom Fe
 line:3 (p) of atom Fe
 line:4 (d) of atom Fe
 line:5 (f) of atom Fe
 line:6 (tot) of atom Se
 line:7 (s) of atom Se
 line:8 (p) of atom Se
 line:9 (d) of atom Se
 line:10 (f) of atom Se
 line:11 (total DOS) of FeSe

Howmany DOS do you want to plot TOGETHER(Max is 4)? 4


Enter line 1 (= lines in FeSe.int)  1
Please enter label 1 : tot Fe

Enter line 2 (= lines in FeSe.int)  4
Please enter label 2 : d Fe

Enter line 3 (= lines in FeSe.int)  6
Please enter label 3 : tot Se

Enter line 4 (= lines in FeSe.int)  11
Please enter label 4 : total DOS
```

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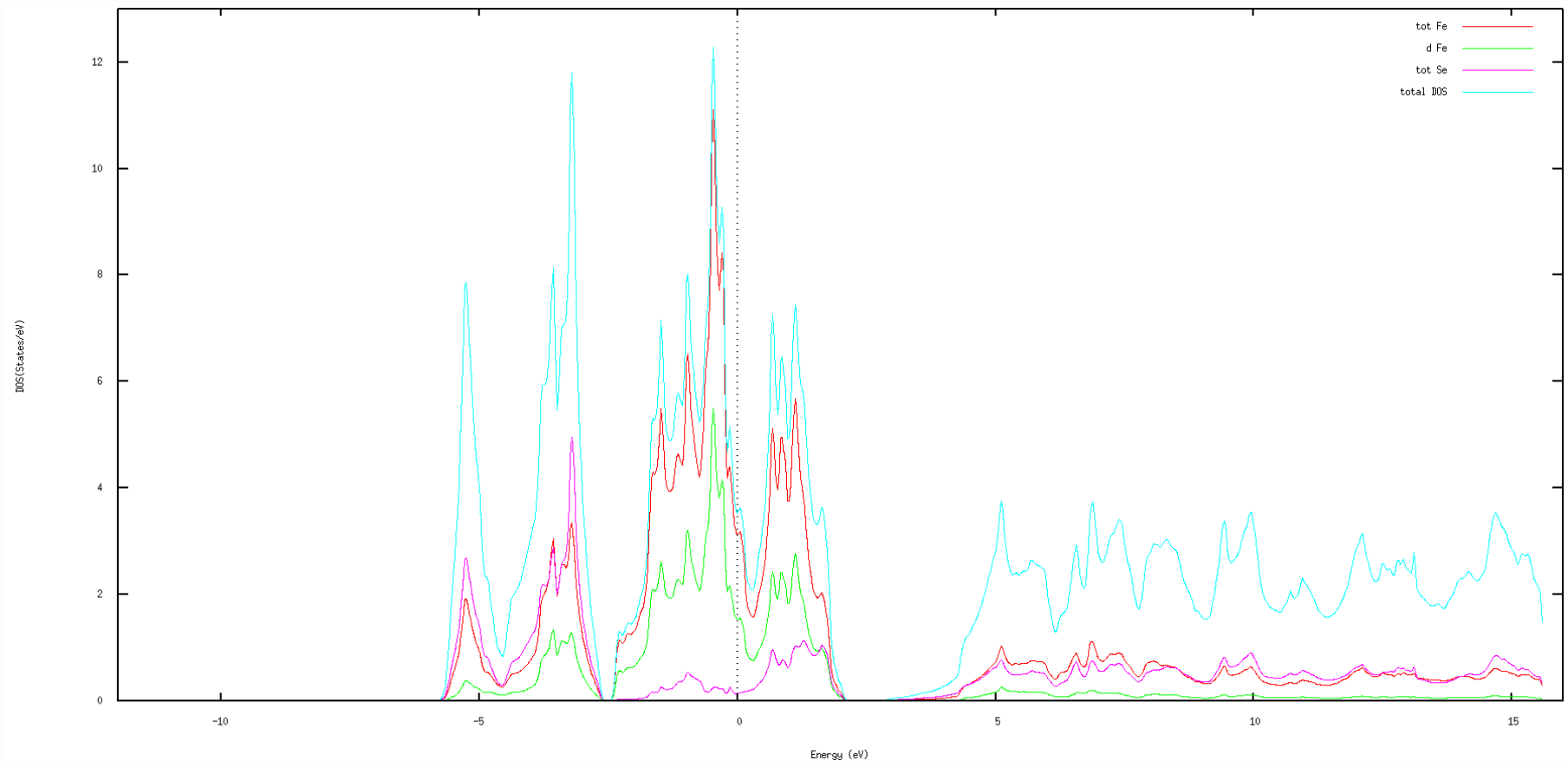
Results of wien2k for FeSe - You should be in the FeSe dir

Density of states



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Wien2k tutorial

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Results of wien2k for FeSe - You should be in the FeSe dir

Density of states

```
Enter line 4 (= lines in FeSe.int)  11
Please enter label 4 : total DOS

Showing partial DOS

Press RETURN to continue

Do you want to set ranges? (y/N)n
Do you want a hardcopy? (y/N)n
[lect10@inter FeSe]$
```

- mkdir FeSe_DOS
- cp * FeSe_DOS

SAVE the DOS calculation

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Results of wien2k for FeSe - **Band Structure**

- cp **$RESULTS/DFT/**FeSe.klist_band
- cp **$RESULTS/DFT/**FeSe.insp

FeSe.insp

```
### Figure configuration
 5.0   3.0                          # paper offset of plot
15.0  22.5                          # xsize,ysize [cm]
 1.0   9                            # major ticks, minor ticks
 1.0   1                            # character height, font switch
 1.1   2    4                       # line width, line switch, color switch
### Data configuration
-1 1 2                              # energy range, energy switch (1:Ry, 2:eV)
2      0.3526254600                 # Fermi switch,  Fermi-level (in Ry units)
1   999                            # number of bands for heavier plotting   1,1
0      1    0.2                     # jatom, jtype, size  of heavier plotting
```

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Results of wien2k for FeSe - **Band Structure**

- grep :FER FeSe.scf

```
[lect10@inter FeSe]$ grep :FER FeSe.scf
:FER  : F E R M I - ENERGY(TETRAH.M.)=   0.3859724178
:FER  : F E R M I - ENERGY(TETRAH.M.)=   0.3860265434
:FER  : F E R M I - ENERGY(TETRAH.M.)=   0.3838682004
:FER  : F E R M I - ENERGY(TETRAH.M.)=   0.3777553652
:FER  : F E R M I - ENERGY(TETRAH.M.)=   0.3562184296
:FER  : F E R M I - ENERGY(TETRAH.M.)=   0.3473916138
:FER  : F E R M I - ENERGY(TETRAH.M.)=   0.3515395363
:FER  : F E R M I - ENERGY(TETRAH.M.)=   0.3515312239
:FER  : F E R M I - ENERGY(TETRAH.M.)=   0.3521528063
:FER  : F E R M I - ENERGY(TETRAH.M.)=   0.3526207866
:FER  : F E R M I - ENERGY(TETRAH.M.)=   0.3526226365
:FER  : F E R M I - ENERGY(TETRAH.M.)=   0.3526254600
[lect10@inter FeSe]$
```

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Results of wien2k for FeSe - **Band Structure**

- emacs -nw FeSe.insp
- Ctrl X, Ctrl S
- Ctrl X, Ctrl C

```
### Figure configuration
 5.0   3.0                          # paper offset of plot
15.0  22.5                          # xsize,ysize [cm]
 1.0   9                            # major ticks, minor ticks
 1.0   1                            # character height, font switch
 1.1   2    4                       # line width, line switch, color switch
### Data configuration
-1 1 2                              # energy range, energy switch (1:Ry, 2:eV)
2      0.3892523284                 # Fermi switch,  Fermi-level (in Ry units)
1   999                            # number of bands for heavier plotting   1,1
0      1    0.2                     # jatom, jtype, size  of heavier plotting
```

```
:FER  : F E R M I - ENERGY(TETRAH.M.)=   0.3526226365
:FER  : F E R M I - ENERGY(TETRAH.M.)=   0.3526254600
[lect10@inter FeSe]$
```

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Results of wien2k for FeSe - **Band Structure**

- **Band Structure**
- x lapw1 –band
- x lapw2 –qtl -band
- x spaghetti

- ls and you should see FeSe.spaghetti_ps

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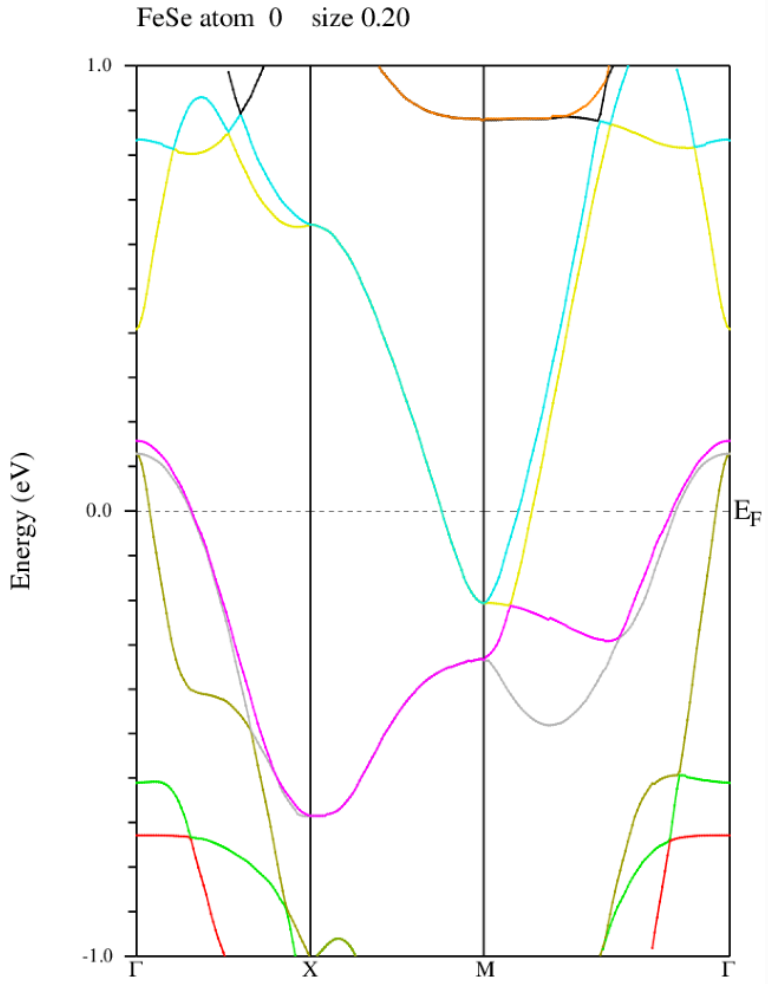
Results of wien2k for FeSe - **Band Structure**

- **Open a new terminal**
- gs FeSe.spaghetti_ps
- xmgrace FeSe.bands.agr
- mkdir FeSe_BANDS
- cp * FeSe_BANDS

SAVE the BAND calculation



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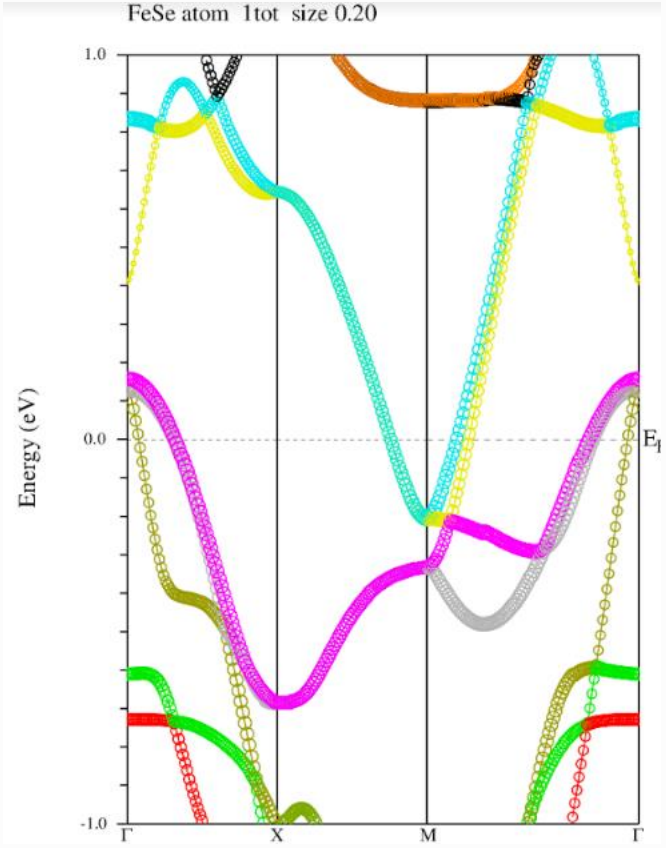
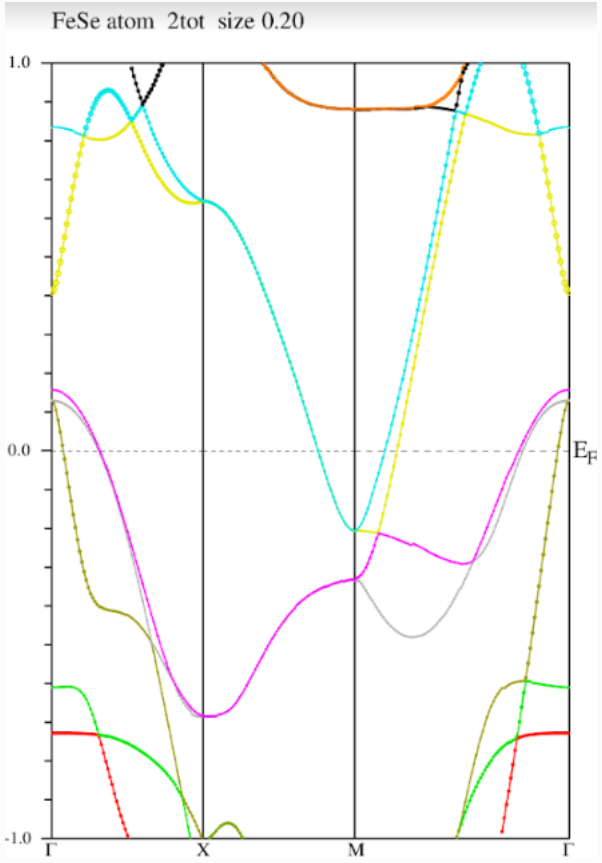
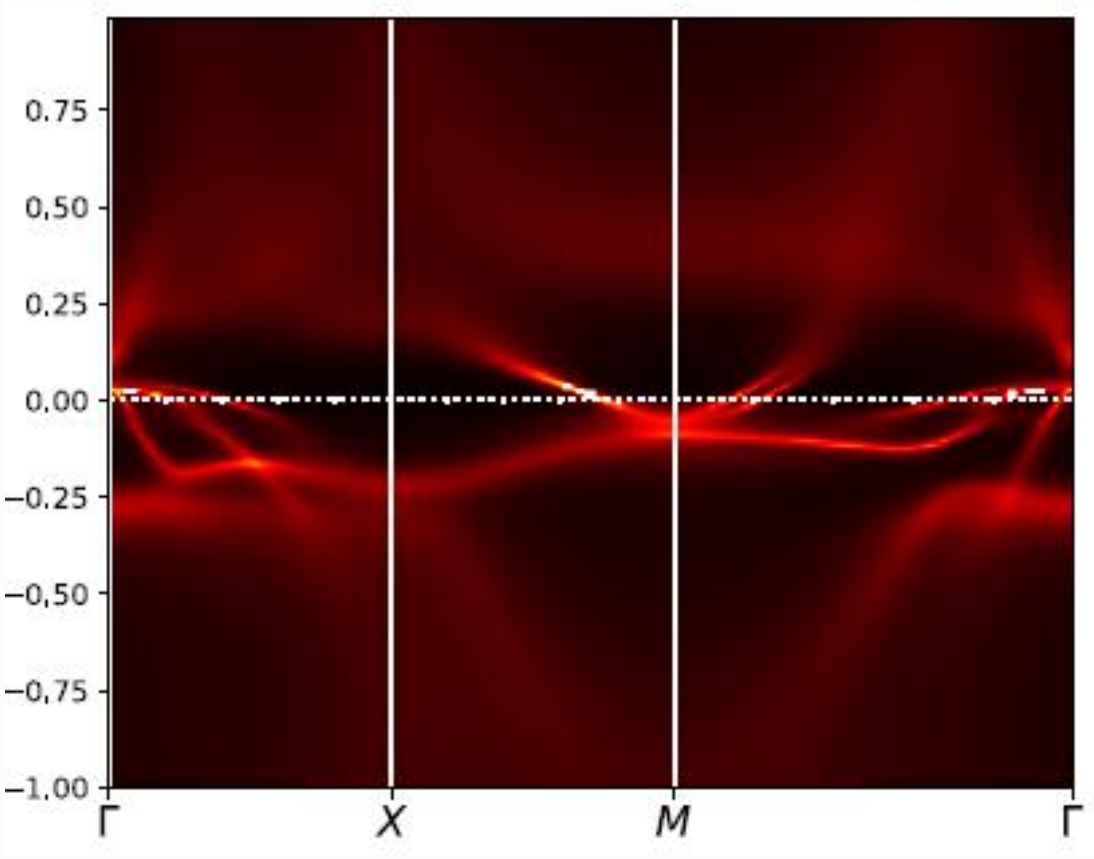
Results of wien2k for FeSe - **Band Structure character**







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Wien2k tutorial

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Results of wien2k for MnO - You should be in the MnO dir

- cd ../MnO
- pwd

```
[lect10@cp1433-mp2 FeSe]$ cd ../MnO
[lect10@cp1433-mp2 MnO]$ pwd
/home/lect10/MnO
[lect10@cp1433-mp2 MnO]$
```

Results of wien2k for MnO

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Wien2k tutorial

Results of wien2k for MnO - You should be in the MnO dir

- grep :CHA MnO.dayfile - energy convergence

run_lapw -ec 0.0001 -cc 0.0001

```
[lect10@cp1433-mp2 MnO]$ grep :CHA MnO.dayfile
:CHARGE convergence:   0 0.0001 0
:CHARGE convergence:   0 0.0001 0
:CHARGE convergence:   0 0.0001 .2970428
:CHARGE convergence:   0 0.0001 .7079523
:CHARGE convergence:   0 0.0001 1.0790402
:CHARGE convergence:   0 0.0001 .2222547
:CHARGE convergence:   0 0.0001 .2048320
:CHARGE convergence:   0 0.0001 .1394405
:CHARGE convergence:   0 0.0001 .1064129
:CHARGE convergence:   0 0.0001 .0300193
:CHARGE convergence:   0 0.0001 .0308621
:CHARGE convergence:   0 0.0001 .0219261
:CHARGE convergence:   0 0.0001 .0101504
:CHARGE convergence:   0 0.0001 .0042793
:CHARGE convergence:   0 0.0001 .0006518
:CHARGE convergence:   0 0.0001 .0004557
:CHARGE convergence:   0 0.0001 .0002238
:CHARGE convergence:   1 0.0001 -.0000399
[lect10@cp1433-mp2 MnO]$
```

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Results of wien2k for MnO - You should be in the MnO dir

- grep :ENE MnO.dayfile - energy convergence

run_lapw -ec 0.0001 -cc 0.0001

```
[lect10@cp1433-mp2 MnO]$ grep :ENE MnO.dayfile
:ENERGY convergence:  0 0.0001 0
:ENERGY convergence:  0 0.0001 0
:ENERGY convergence:  0 0.0001 .0264068500000000
:ENERGY convergence:  0 0.0001 .0170616550000000
:ENERGY convergence:  0 0.0001 .1368756100000000
:ENERGY convergence:  0 0.0001 .0984619900000000
:ENERGY convergence:  0 0.0001 .0801456300000000
:ENERGY convergence:  0 0.0001 .0013164050000000
:ENERGY convergence:  0 0.0001 .0015890200000000
:ENERGY convergence:  0 0.0001 .0022623150000000
:ENERGY convergence:  0 0.0001 .0008895050000000
:ENERGY convergence:  1 0.0001 .0000734900000000
:ENERGY convergence:  1 0.0001 .0000778950000000
:ENERGY convergence:  1 0.0001 .0000406400000000
:ENERGY convergence:  1 0.0001 .0000132400000000
:ENERGY convergence:  1 0.0001 .0000054150000000
:ENERGY convergence:  1 0.0001 .0000046950000000
:ENERGY convergence:  1 0.0001 .0000006300000000
[lect10@cp1433-mp2 MnO]$
```

SAVE the calculation for DMFT

- mkdir MnO
- cp * **MnO**

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Results of wien2k for MnO - You should be in the MnO dir

- **Density of states**
- x kgen put 5000
- x lapw1
- x lapw2 –qtl

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Results of wien2k for MnO - You should be in the MnO dir

- **Density of states**
- configure_int_lapw
- x tetra

```
[lect10@cp1433-mp2 MnO]$ configure_int_lapw
     (C)2008 by Morteza Jamal
#####################################
#                                   #
 Configures and creates MnO.int
#                                   #
#####################################

atom 1 is Mn
atom 2 is O

*** For Total DOS type 'total' ***

*** For finishing type 'end' ***

Please enter the number of atom that you like to plot DOS? (default:1) 1
Select PDOS for Mn from: tot,s,p,d,d-eg,d-t2g,f (give a comma-separated list).
tot,s,p,d,f

*** For finishing type 'end' ***

Please enter the number of atom that you like to plot DOS? (default:2) 2
Select PDOS for O from: tot,s,p,d,d-eg,d-t2g,f (give a comma-separated list).
tot,s,p,d,f

*** For finishing type 'end' ***

Please enter the number of atom that you like to plot DOS? (default:3) total

*** For finishing type 'end' ***

Please enter the number of atom that you like to plot DOS? (default:4) end

MnO.int is ready for using.

[lect10@cp1433-mp2 MnO]$
```

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Results of wien2k for MnO - You should be in the MnO dir

- **Density of states**
- **Open a new terminal**
- dosplot2

```
*ATTENTION*
You can select 11 + 0  DOS for plotting in MnO.int .

Please see and select lines to plot.

 line:1 (tot) of atom Mn
 line:2 (s) of atom Mn
 line:3 (p) of atom Mn
 line:4 (d) of atom Mn
 line:5 (f) of atom Mn
 line:6 (tot) of atom O
 line:7 (s) of atom O
 line:8 (p) of atom O
 line:9 (d) of atom O
 line:10 (f) of atom O
 line:11 (total DOS) of MnO

Howmany DOS do you want to plot TOGETHER(Max is 4)? 4


Enter line 1 (= lines in MnO.int)  1
Please enter label 1 : tot Mn

Enter line 2 (= lines in MnO.int)  4
Please enter label 2 : d Mn

Enter line 3 (= lines in MnO.int)  6
Please enter label 3 : tot O

Enter line 4 (= lines in MnO.int)  11
Please enter label 4 : total DOS

Showing partial DOS

Press RETURN to continue
```

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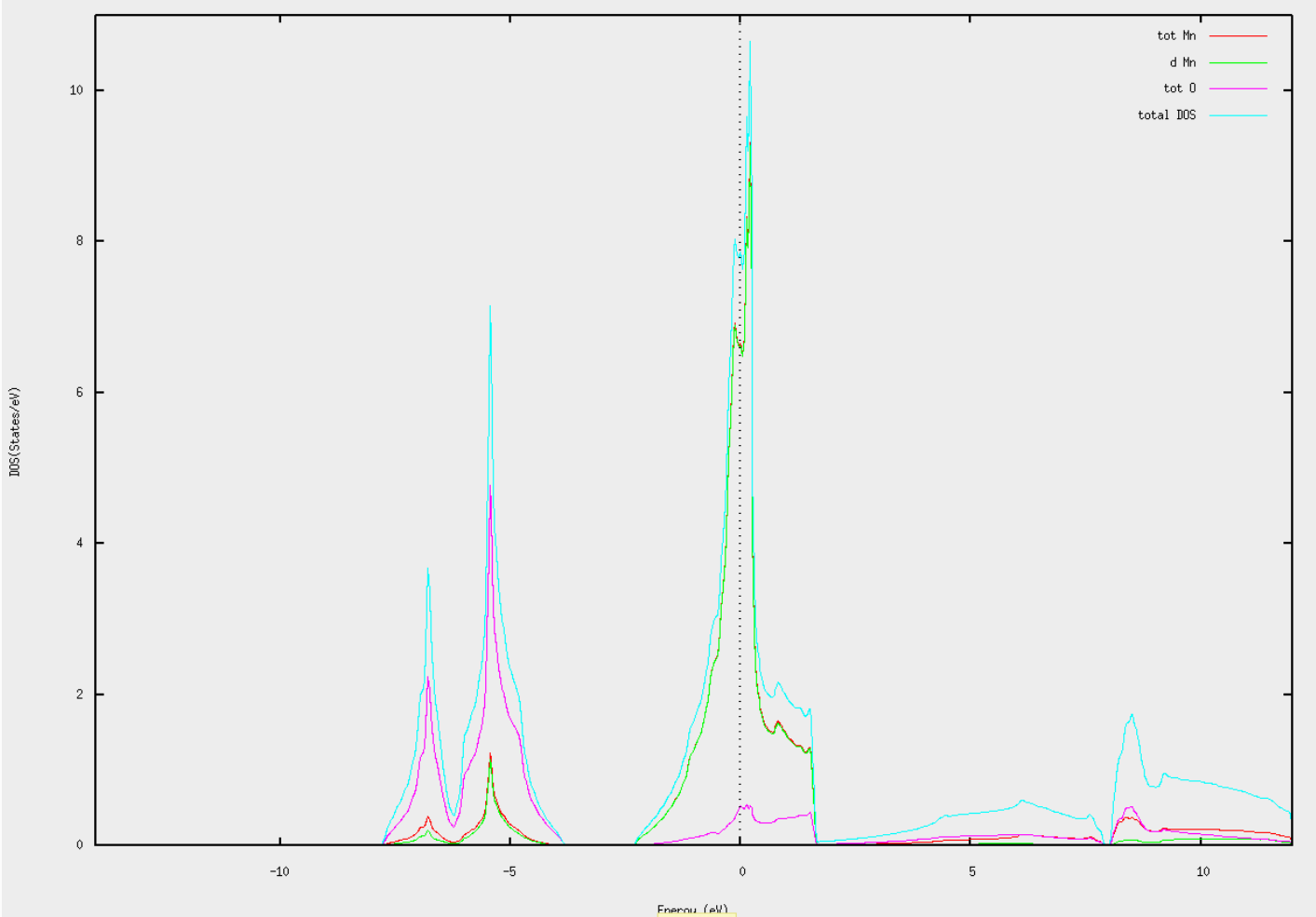
Results of wien2k for MnO - You should be in the MnO dir

- **Density of states**



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Wien2k tutorial

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For any questions related to this talk PLEASE email

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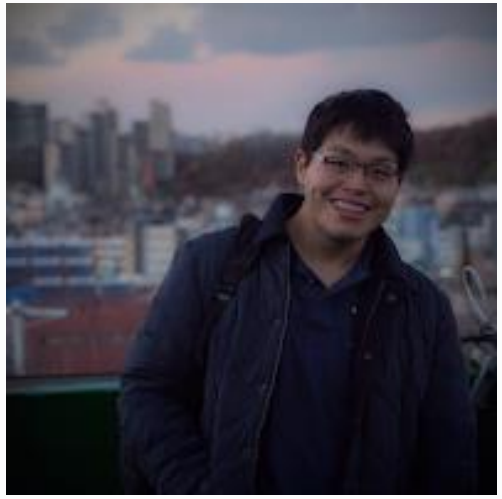

Thank you very much for your attention!

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