Winter School *Computational* Magnetism

VASP Tutorial

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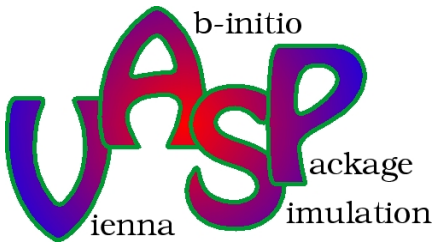


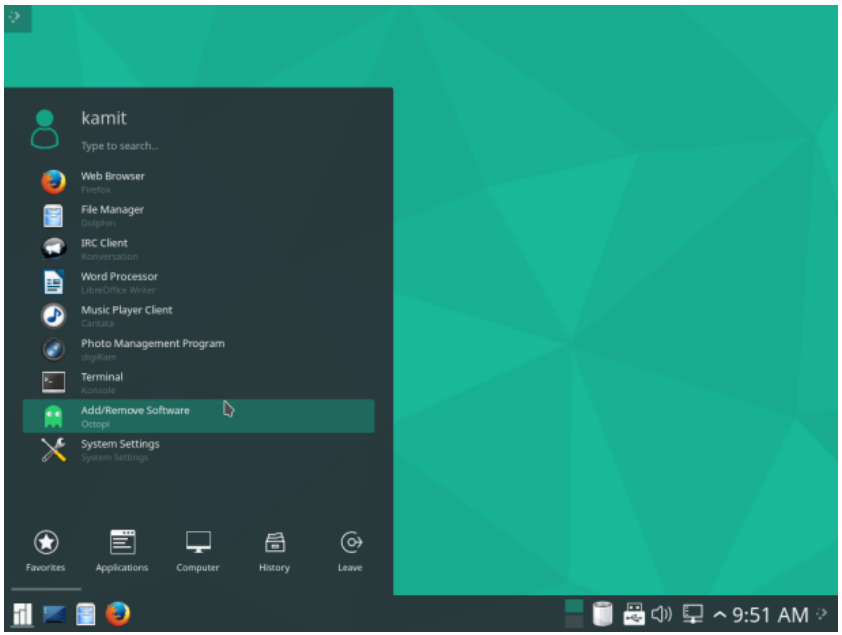
Outline

- Login
- VASP
- Exercises

Login on PC

1. Each PC is associated with a number from 01 to 29, let's label it: ##
2. login on your PC

   username: `training`
   password: `Vicom_2017`
3. Open a terminal window on your PC:



Login

1. From the terminal login to VSC:
   `ssh -X vsc3.vsc.ac.at` password: Vicom_2017

2. Go to your working directory
   `cd ##/vasp` mind ##=your PC number [01-29]

   Type `ls`. Find 4 directories (one for each exercise) and a readme file:
   `01_Nifcc` `02_MnO` `03_Fefcc` `04_CoO` `readme.txt`

   You can open `readme.txt` with any editor: nano, vi, emacs

3. To run the examples it is necessary login to a compute node.
   i. Allocate one compute node:
      `salloc -J pc##`
   ii. Find which node has been allocated
      `node`
   iii. Login to allocated node:
      `ssh -X` 'output of `node`' (i.e. ssh -X n41-005)
   iv. `cd ##/vasp`
   v. Ready to run the examples!

VASP: input files

VASP requires the following input files:

- INCAR: central input file, it determines 'what to do and how to do it' (many parameters: refer to VASP manual).
- KPOINTS: contains the k-point coordinates and weights or the mesh size for creating the k-point grid.
- POSCAR: contains the lattice geometry and the ionic positions.
- POTCAR: contains the atomic pseudopotential.

$\Rightarrow$ All inputs files are already available in your directories

VASP: output files

The main output files:

- OUTCAR: central output file.
- vasprun.xml: output data
  Can be open with the graphical interface P4Vasp

  ```
  p4v vasprun.xml
  ```

  (vasprun.xml can be renamed: `p4v newname.xml`)

VASP inputs; Example 01 (01Nifcc)

POSCAR

```
fcc Ni                  –> Title
3.524                   –> Lattice constant
0.5 0.5 0.0             –> Bravais Matrix (in this case FCC)
0.0 0.5 0.5
0.5 0.0 0.5
Ni                      –>Atom Type
1                       –> Number of atoms
cartesian               –> Type of coordinates: cartesian or direct
0 0 0                   –> atom positions (x, y, z)
```

VASP inputs; Example 01 (01Nifcc)

Refer to online VASP manual for detailed description of flags

INCAR

```
System = fcc Ni
ISTART = 0          -> start from scratch
ISMEAR = -5         -> integration method in reciprocal space
ISPIN = 2           -> spin-polatized calculation, 2 spins
MAGMOM = 1.0        -> Initial magnetic moment
```

VASP inputs; Example 01 (01Nifcc)

KPOINTS

```
K-Points                 –> Title
0                        –> Number of k-points (0 = automatic generation)
Monkhorst Pack           –> Type of grid
11 11 11                 –> subdivisions along reciprocal lattice vectors
0 0 0                    –> Optional shift
```

VASP inputs; Example 01 (01Nifcc)

POTCAR

```
PAW_PBE Ni 06Sep2000
10.00000000000000000
parameters from PSCTR are:
VRHFIN =Ni:
LEXCH = PE
...
```

Exercises

1. fcc Ni
   1. Simple FM element: Volume, DOS & Bands
   2. Energy as a function of the size of the magnetic moment.
2. MnO
   1. AFM ordering: moment and gap using DFT, DFT+U & HSE
   2. Nearest-neighbour exchange parameter J_1
3. Spin spirals in fcc Fe
4. Magnetic Anisotropy Energy (MAE) in strained CoO

Exercises: howto RUN

All exercises can be run with available `shell scripts`:

1. fcc Ni
   1. Simple FM element: Volume, DOS & Bands
      `00_volume.sh` `01_dos.sh` `02_bands.sh`
   2. Energy as a function of the size of the magnetic moment.
      `magmom.sh`
2. MnO
   1. AFM ordering: moment and gap using DFT, DFT+U & HSE
      `dos.sh`
   2. Nearest-neighbour exchange parameter J_1
      `j.sh`
3. Spin spirals in fcc Fe
   `spirals.sh`
4. Magnetic Anisotropy Energy (MAE) in strained CoO
   `mae.sh`

Exercises: howto VISUALIZE

All results can be visualized using:

1. `p4v`

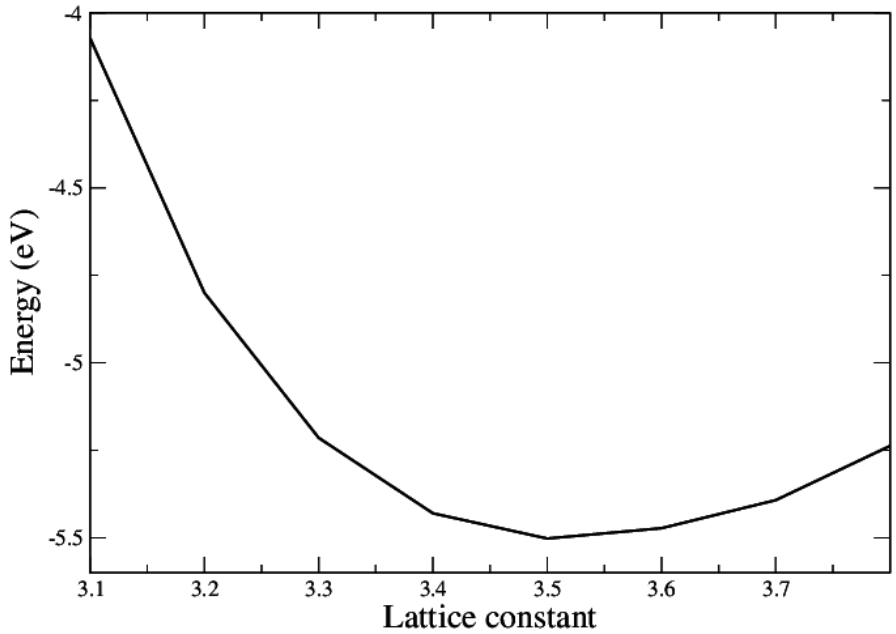
   VASP graphical interface: see www.p4vasp.at

2. `xmgrace` or `gnuplot`

3. open OUTCAR file with some editors

Exercise 01: 01_Nifcc/01/

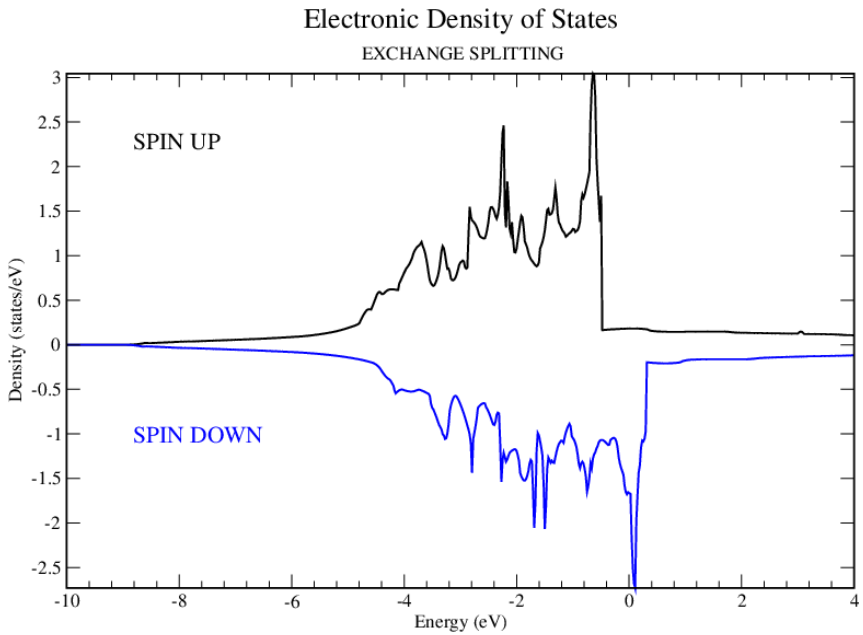
1. `./00_volume.sh`
2. `xmgrace volume.dat`
3. Output



minimum at $a \sim 3.542$

Exercise 01: 01_Nifcc/01/

1. `./01_dos.sh`
2. `p4v` (click DOS+bands)
3. Output



minimum at $a \sim 3.542$

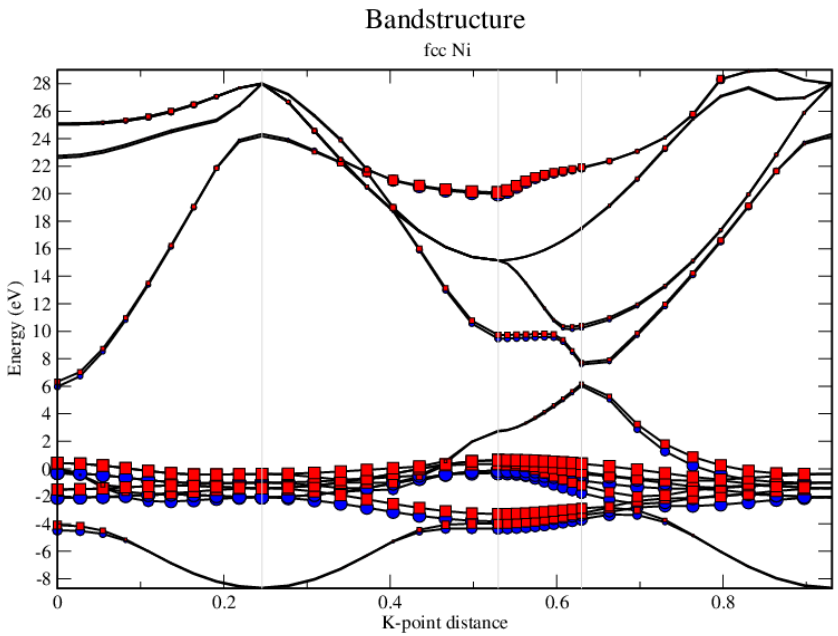
Exercise 01: 01_Nifcc/01/

Value of spin moment written in OUTCAR

```
  magnetization (x)

# of ion       s       p       d       tot
------------------------------------------------
  1        -0.007  -0.027   0.635   0.600

   total charge

# of ion       s       p       d       tot
------------------------------------------------
  1         0.495   0.490   8.326   9.311
```

Exercise 01: 01_Nifcc/01/

1. `./02_bands.sh`
2. `p4v` (click DOS+bands –> Show-Bands)
3. Output



Exercise 01: 01_Nifcc/02/

Goal: Total energy vs. magnetic moment

How: Constrained magnetic moment calculations

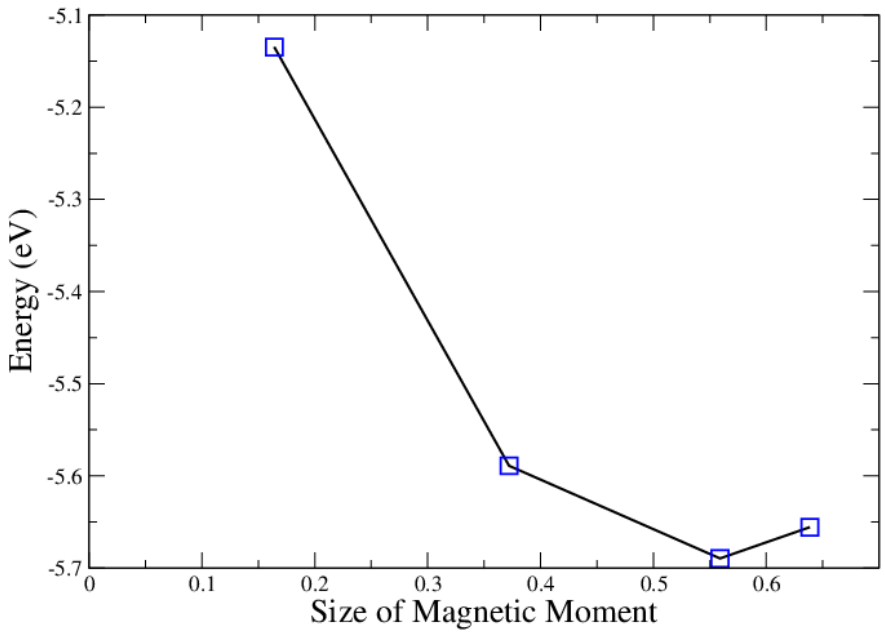
Flags in INCAR:

```
LNONCOLLINEAR = .TRUE.
SAXIS = 0 0 1
RWIGS = 1.0
I_CONSTRAINED_M=2 (constrain direction & size)
M_CONSTR = 0 0 size (x, y, z components of magmom)
LAMBDA = 20
```

the script will compute the energy for different value of 'size'

Exercise 01: 01_Nifcc/02/

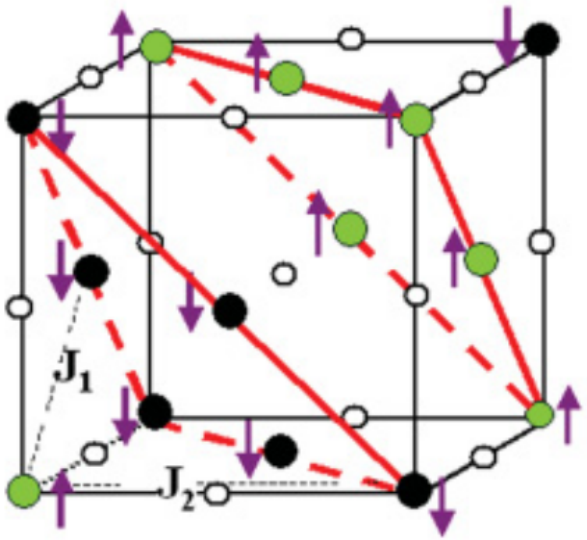
1. `./magmom.sh`
2. `xmgrace mag_energy.dat`
3. Output



in agreement with PRL 77 334 (1996)

Exercise 02: 02_MnO/01_AFMII

Goal: DOS for AFM-II ordered MnO at different level of theory



AF2: A-type (111)

MnO: 'cubic' rock-salt structure with spins AFM aligned along 111

How (1): AFM ordering, 4 atoms unit cell (`p4v` POSCAR –> show)

```
ISPIN     = 2
MAGMOM    = 5.0 -5.0 0 0
```

How (2): PBE, PBE+U and HSE (Hybrid functionals)

DFT+U

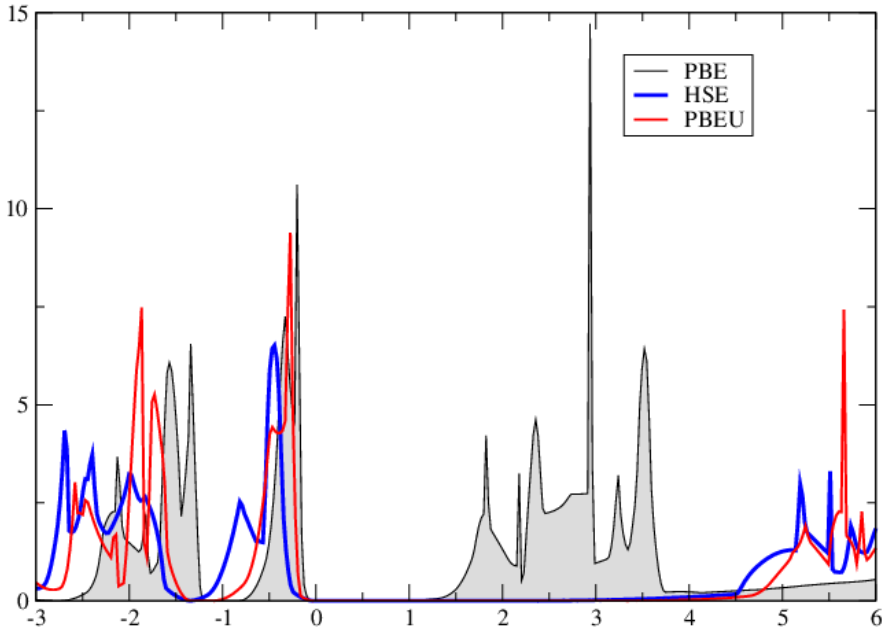
```
LDAU       = .TRUE.
LDAUTYPE   = 2
LDAUL      = 2 -1
LDAUU      = 7.00 0.00
LDAUJ      = 1.00 0.00
LDAUPRINT  = 2
```

HSE

```
LHFCALC = .TRUE.
ALGO = All ; TIME = 0.4
HFSCREEN = 0.2
PRECFOCK  = Fast
NKRED = 2
```

Exercise 02: 02_MnO/01_AFMII

1. `./dos.sh`
2.
```
p4v vasprun_pbe.xml
p4v vasprun_pbe+u.xml
p4v vasprun_hse.xml
```
3. Output



Experimental gap $\approx$ 4 eV

Exercise 02: 02_MnO/01_AFMII

Goal: Compute J_1 by total energy differences (per f.u.)

To extract J_1 and J_2 we fit our calculated total energies to a standard two-parameter classical Heisenberg Hamiltonian of the following form:

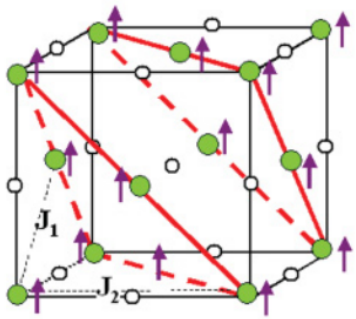
$$H = -J_1 \sum_{\langle i,j \rangle} \vec{e}_i \cdot \vec{e}_j - J_2 \sum_{\langle\langle i,j \rangle\rangle} \vec{e}_i \cdot \vec{e}_j,$$

where $\langle i,j \rangle$ and $\langle\langle i,j \rangle\rangle$ indicate summation over NN and NNN, respectively, and $\vec{e}_i$ is the spin direction unit vector. Energies (per f.u.) are then expressed as:

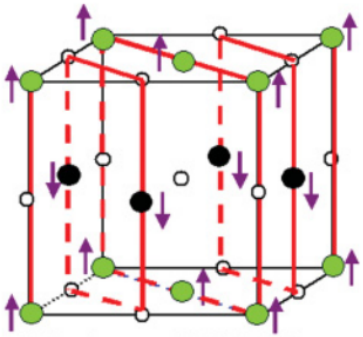
$$E_{\mathrm{FM}} = E_0 - 6J_1 - 3J_2,$$
$$E_{\mathrm{AF_1}} = E_0 + 2J_1 - 3J_2,$$
$$E_{\mathrm{AF_2}} = E_0 + 3J_2.$$

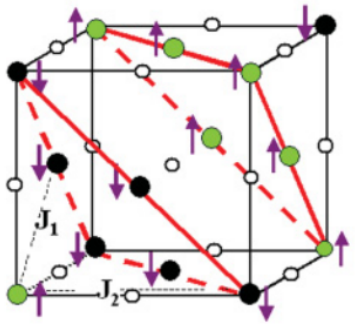
This is solved to give:

$$J_1 = \tfrac{1}{8}\left(E_{\mathrm{AF_1}} - E_{\mathrm{FM}}\right),$$
$$J_2 = \tfrac{1}{24}\left(4E_{\mathrm{AF_2}} - 3E_{\mathrm{AF_1}} - E_{\mathrm{FM}}\right).$$



FM


AF1: A-type (001)/(110)

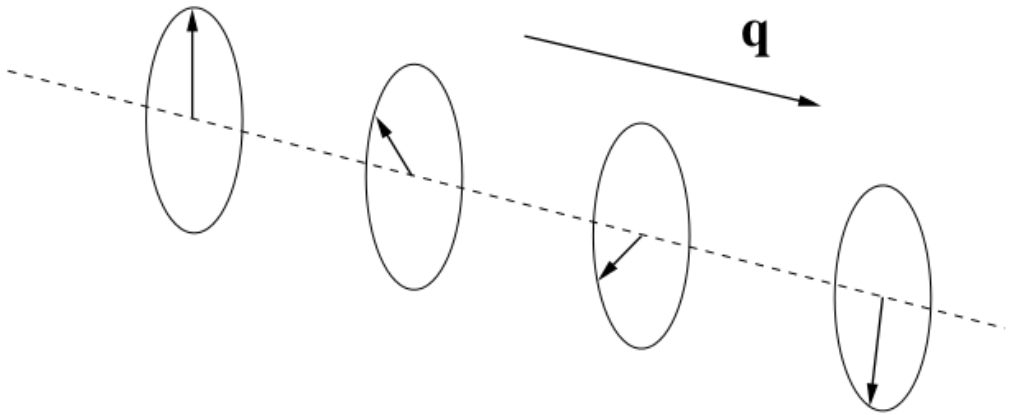


AF2: A-type (111)

How: $J_1 = 1/8(E_{AFI} - E_{FM})$, check INCAR and POSCAR file!

`./j.sh` output: 9.39 meV, in agreement with PRB 84 115114 2011

Spin spirals



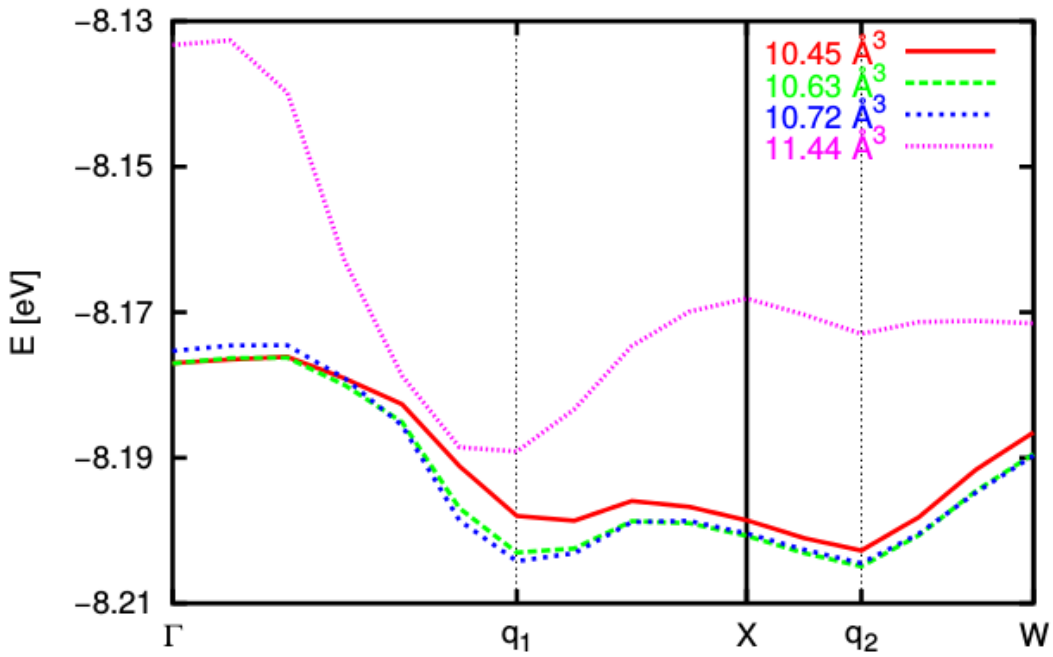
$$\mathbf{m}(\mathbf{r}+\mathbf{R}) = \begin{pmatrix} m_x(\mathbf{r})\cos(\mathbf{q}\cdot\mathbf{R}) - m_y(\mathbf{r})\sin(\mathbf{q}\cdot\mathbf{R}) \\ m_x(\mathbf{r})\sin(\mathbf{q}\cdot\mathbf{R}) + m_y(\mathbf{r})\cos(\mathbf{q}\cdot\mathbf{R}) \\ m_z(\mathbf{r}) \end{pmatrix}$$

Generalized Bloch condition

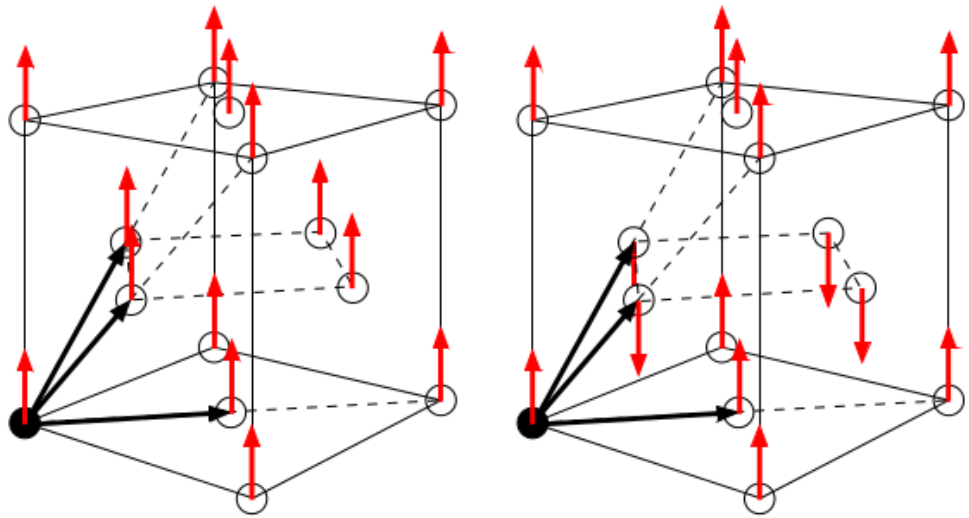
$$\begin{pmatrix} \Psi^{\uparrow}_{\mathbf{k}}(\mathbf{r}) \\ \Psi^{\downarrow}_{\mathbf{k}}(\mathbf{r}) \end{pmatrix} = \begin{pmatrix} e^{-i\mathbf{q}\cdot\mathbf{R}/2} & 0 \\ 0 & e^{+i\mathbf{q}\cdot\mathbf{R}/2} \end{pmatrix} \begin{pmatrix} \Psi^{\uparrow}_{\mathbf{k}}(\mathbf{r}-\mathbf{R}) \\ \Psi^{\downarrow}_{\mathbf{k}}(\mathbf{r}-\mathbf{R}) \end{pmatrix}$$

Spin spirals in fcc Fe

$$\Gamma\,(\mathrm{FM}) = \frac{2\pi}{a_0} \times (0,0,0)$$
$$\mathbf{q_1} = \frac{2\pi}{a_0} \times (0,0,0.6)$$
$$\mathrm{X}\,(\mathrm{AFM}) = \frac{2\pi}{a_0} \times (0,0,1.0)$$
$$\mathbf{q_2} = \frac{2\pi}{a_0} \times (0.15,0,1.0)$$



$$\mathbf{q}_{\mathrm{exp}} = \frac{2\pi}{a_0} \times (0.1,0,1.0)$$

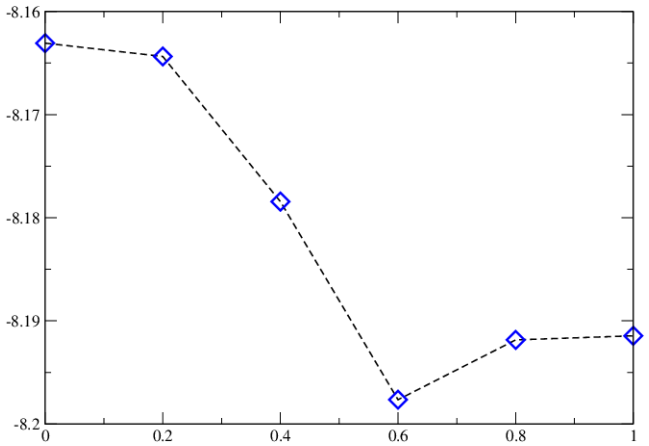


How: LSPIRALS & QSPIRALS in INCAR

```
LNONCOLLINEAR = .TRUE.
MAGMOM  = 3.0 0.0 0.0

LSPIRAL = .TRUE.
QSPIRAL = 0.5 0.00 0.5    = 2pi/a(0,0,1)
LZEROZ  = .TRUE.
```

```
./spirals.sh
```

```
xmgrace energies_GX.dat
```



Exercise 04: 04_CoO

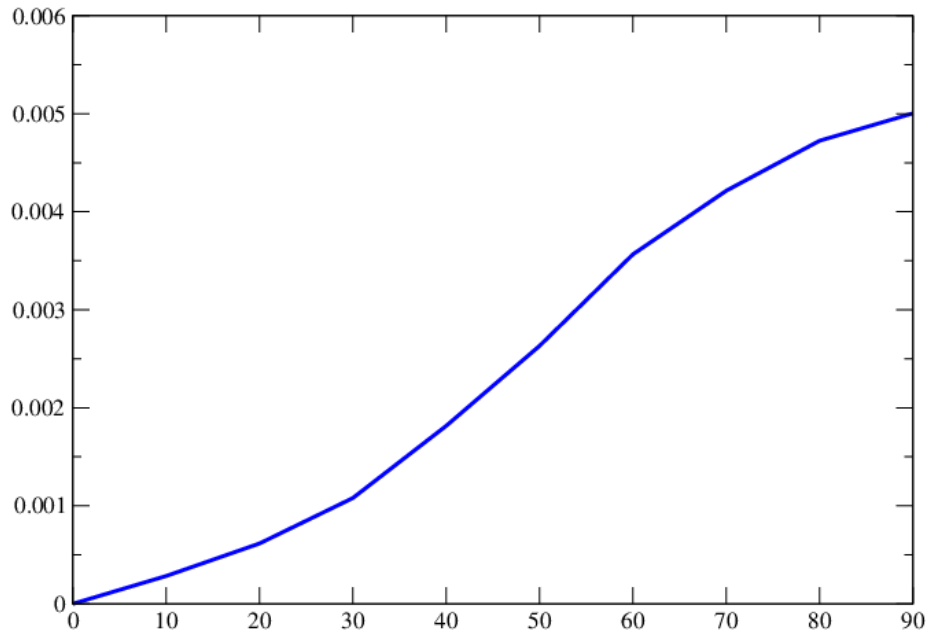
Goal: MAE in strained CoO-AFII, PRL 95 187205 (2005)

How: Constrain direction only of magnetic moment

```
LNONCOLLINEAR = .TRUE.
SAXIS = 0 0 1
#          x1 y1 z1 x2 y2 z2 x3 y3 z3 x4 y4 z4
#MAGMOM = 0   0   3   0   0 -3   0   0   0   0   0   0 # 0
#MAGMOM = 3   0   0   3   0   0   0   0   0   0   0   0 #90

I_CONSTRAINED_M=1
RWIGS = 1.302 0.900
#M_CONSTR = 0   0   3   0   0 -3   0 0 0 0 0 0 # 0
#M_CONSTR = 3   0   0   3   0   0   0 0 0 0 0 0 #90
```

Exercise 04: 04_CoO

1. `./mae.sh`
2. `xmgrace MAE.dat`



Exercise 04: 04_CoO

Large orbital moment (LORBMOM = .TRUE.)

In OUTCAR (90 deg):

```
 orbital moment (x)

# of ion       p       d       tot
------------------------------------
  1        -0.000   0.173   0.173
  2         0.000  -0.173  -0.173
  3         0.000   0.000   0.000
  4         0.000   0.000   0.000
------------------------------------
            0.000   0.000   0.000
```

Exercise 04: 04_CoO

Spin moment, in OUTCAR (90 deg):

magnetization (x)

# of ion	s	p	d	tot
1	0.006	-0.005	2.285	2.286
2	-0.006	0.005	-2.284	-2.285
3	-0.000	0.000	0.000	0.000
4	-0.000	0.000	0.000	0.000
tot	0.000	0.000	0.002	0.002