Workshop and International Conference on

Electronic Structure Theory of
Emergent Spin Orbit Driven Phenomenon

Tutorial 3: Magnetism using DFT - Magnetic ground states and anisotropy

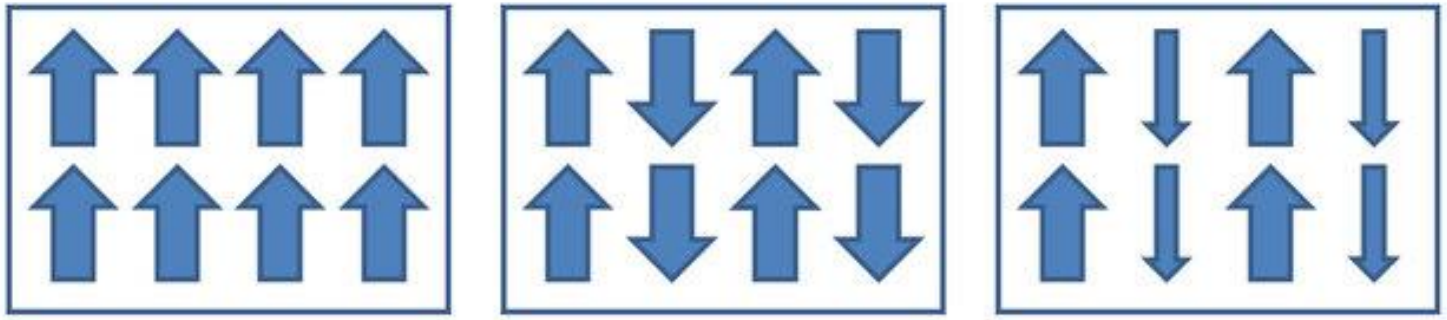
Junaid Jami

Magnetic Calculations

1. Find the magnetic ground state of Fe

Taking the ferromagnetic, ferrimagnetic and anti-ferromagnetic configurations

Magnetic Ordering



Ferromagnetism	Anti-ferromagnetism	Ferrimagnetism
FM	AFM	FiM
Fe, Co, Ni	Cr, NiO, Fe_2O_3	$Fe^{2+}Fe_2^{3+}O_4$ (Magnetite), Ferrites

Magnetization → FM > FiM > AFM

For AFM → Magnetization is zero

Login details

PC login password: student

WiFi details:

U: estesodp.guest1

p: Hks3U$M

Server IP: 10.111.1.12
User Name: estesodp.g1/2/3/4
password: tut_estesodp_2024

Use secure shell to connect to cluster

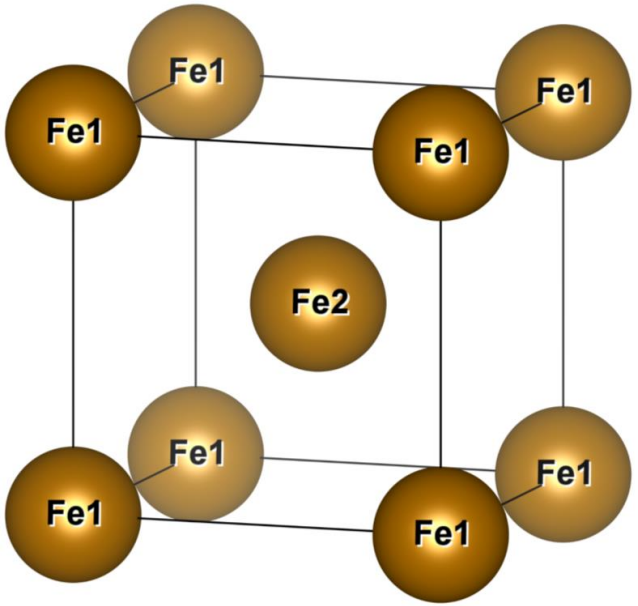
ssh estesodp@10.111.1.12

or ssh -oHostKeyAlgorithms=+ssh-dss estesodp@10.111.1.12

Fe POSCAR

1. Login to the cluster
2. Open folder Tut_3
3. Go to Fe folder
4. Copy POSCAR to your local system
5. Open POSCAR in VESTA

Server IP: 10.111.1.12
User Name: estesodp.g1/2/3/4
password: tut_estesodp_2024



Basic input for magnetic materials

ISPIN = 2 and MAGMOM = NIONS*Magnetic Moment

Get from **POSCAR** file

```
Fe_bcc
1.0
   2.863054989499160    0.000000000000000    0.000000000000002
   0.000000000000005    2.863054989499160    0.000000000000002
   0.000000000000000    0.000000000000000    2.863054989499160
Fe
2
direct
   0.000000000000000    0.000000000000000    0.000000000000000
   0.500000000000000    0.500000000000000    0.500000000000000
```

Basic input for magnetic materials

ISPIN = 2 and MAGMOM = NIONS*Magnetic Moment

↓

Get from **POSCAR** file

Tip: To converge to the magnetic ground state, we recommend setting the magnetic moments slightly larger than the expected values, e.g., using the experimental magnetic moment multiplied by 1.2 or 1.5.

- The final magnetic state strongly depends on the initial values for MAGMOM.[1]

- Fe – 2.2 μ_B (Experimental)

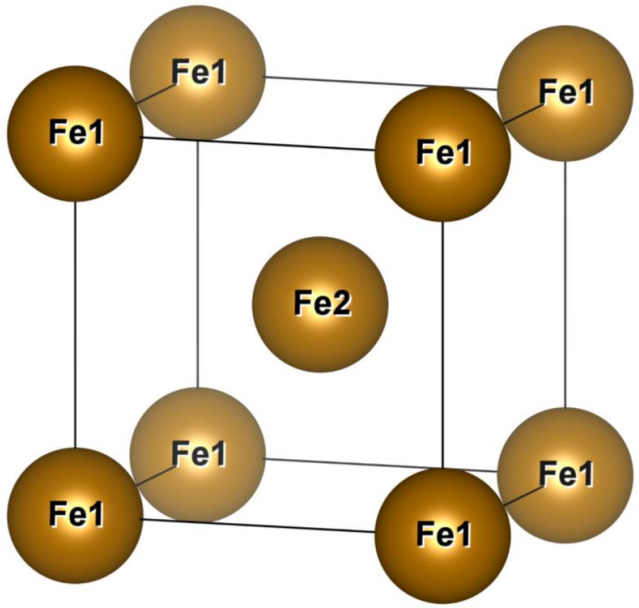
density functional theory - What's the difference between spin-unpolarized, spin-polarized and non-colinear calculation? - Matter Modeling Stack Exchange

1. Huensch et al., PRX 11, 011031 (2021)

INCAR for magnetic material : Fe

INCAR for non-magnetic metal

```
ISTART=0
ISMEAR = 1
SIGMA = 0.2
ENCUT = 500
IBRION =2
NSW =300
ISIF=3
EDIFF = 0.1E-05
EDIFFG = -0.001
LORBIT = 11
PREC = Accurate
```

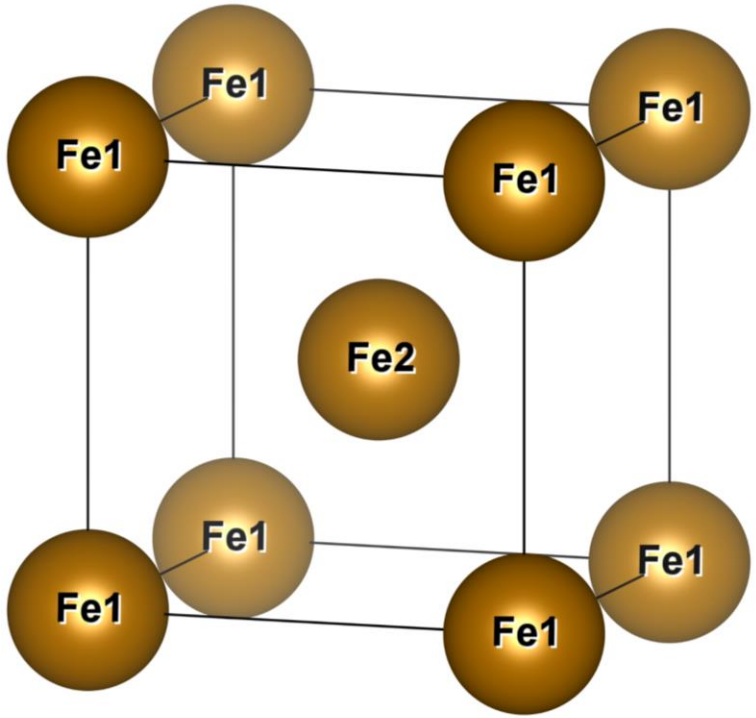


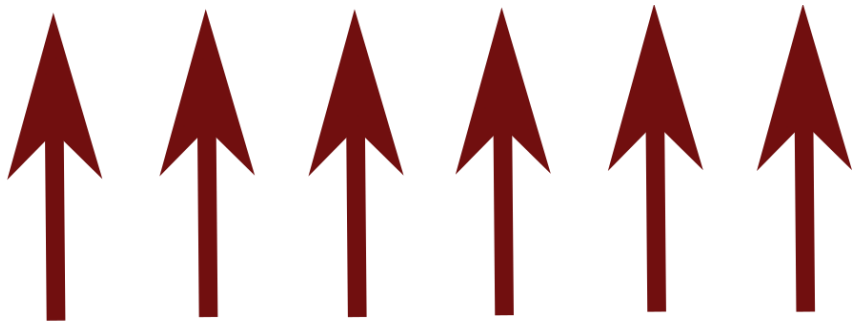

```
ISTART=0
ISMEAR = 1
SIGMA = 0.2
ENCUT = 500
IBRION =2
NSW =300
ISIF=3
EDIFF = 0.1E-05
EDIFFG = -0.001
LORBIT = 11
PREC = Accurate
ISPIN=2
MAGMOM = 2*4
```

Ferromagnetism

Maximum magnetic moment

All moments in same direction





Spin up = positive

NIONS = 2

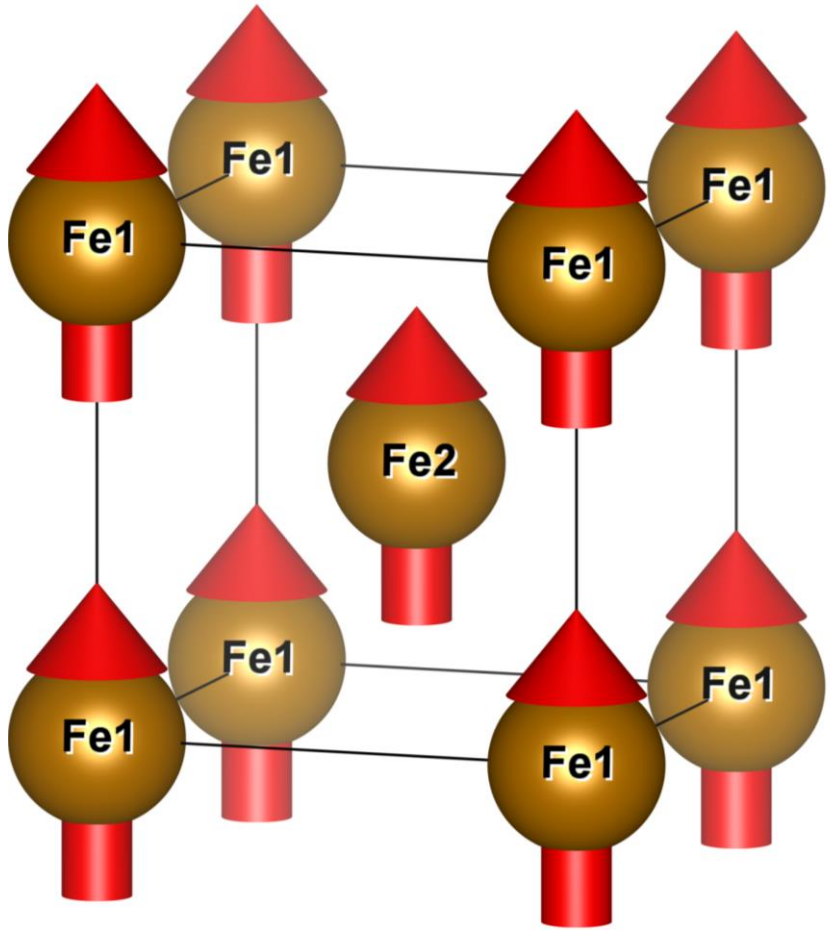
MAGMOM = 2*4

INCAR for bcc Fe – FM configuration

```
ISTART=0
ISMEAR = 1
SIGMA = 0.2
ENCUT = 500
IBRION =2
NSW =300
ISIF=3
EDIFF = 0.1E-05
EDIFFG = -0.001
LORBIT = 11
PREC = Accurate
ISPIN=2
MAGMOM = 2*4
```

Calculation 1 :
Tut_3/Fe/relax_scf/input

qsub job.sh



MAGMOM = 2*4

OUTCAR

```
 magnetization (x)

# of ion       s       p       d       tot
--------------------------------------------
    1        -0.011  -0.048   2.262   2.203
    2        -0.011  -0.048   2.262   2.203
--------------------------------------------
tot          -0.023  -0.096   4.525   4.406
```

Atom-wise magnetic moment and the total magnetic moment

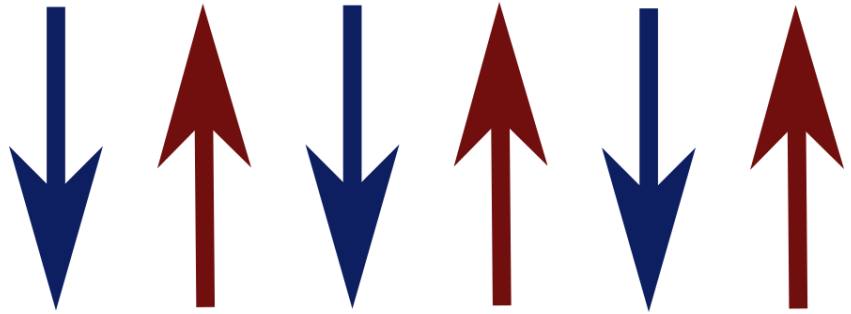
Orbital-wise contribution to magnetic moments

```
FREE ENERGIE OF THE ION-ELECTRON SYSTEM (eV)
---------------------------------------------------
free  energy   TOTEN  =       -16.47327343 eV
```

TOTEN for FM = -16.47327343 eV

Antiferromagnetism

- Complete cancellation of magnetic moments
- Between same atoms only
- M atom can cancel M atom, M atom cannot cancel N atom



Spin up = positive
Spin down = negative

For Fe (2 atoms) = 1 up + 1 down

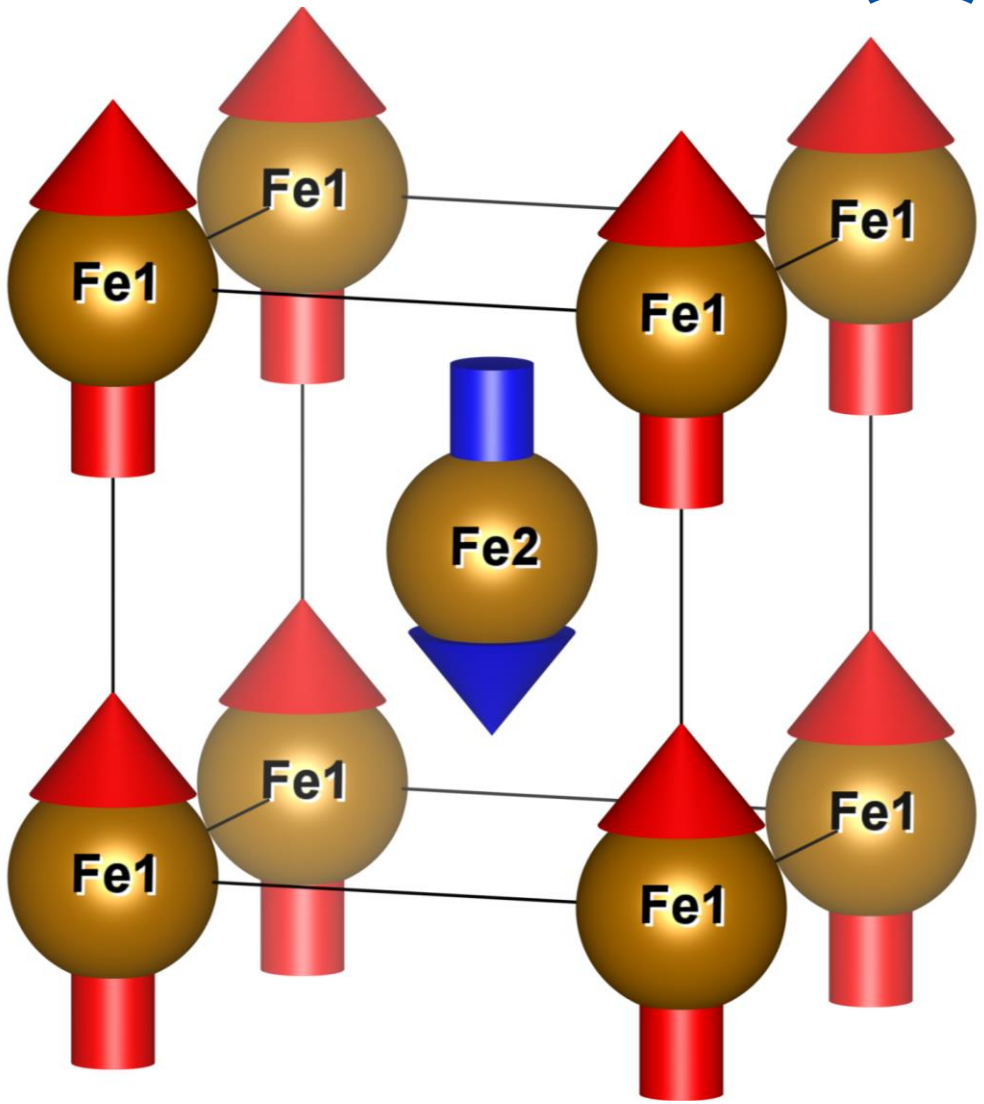
MAGMOM = 1*4 1*-4

INCAR

```
ISTART=0
ISMEAR = 1
SIGMA = 0.2
ENCUT = 500
IBRION =2
NSW =300
ISIF=3
EDIFF = 0.1E-05
EDIFFG = -0.001
LORBIT = 11
PREC = Accurate
ISPIN=2
MAGMOM = 1*4 1*-4
```

Calculation 2 :
Tut_3/Fe/AFM/input

qsub
job.sh

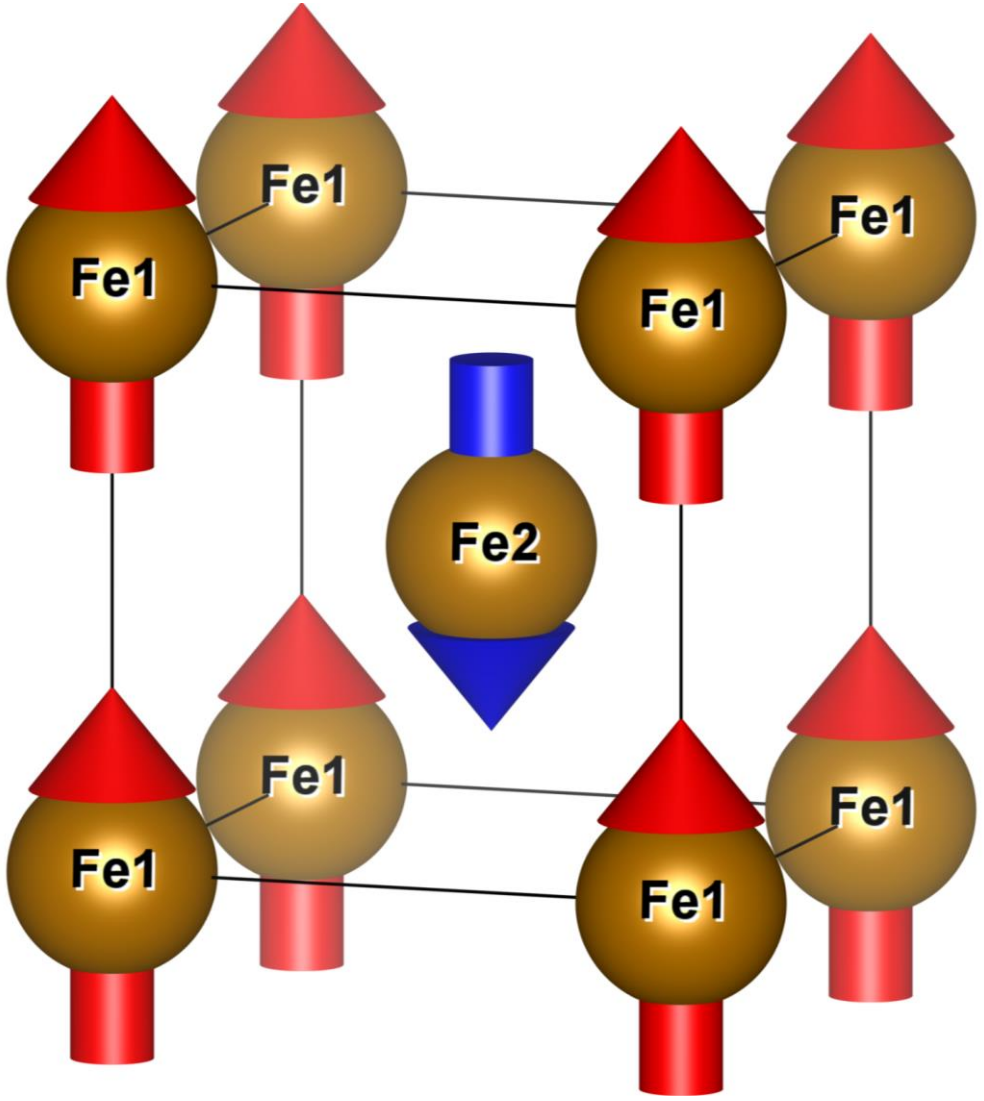


OUTCAR

```
 magnetization (x)

# of ion       s       p       d       tot
--------------------------------------------
    1        0.015   0.023   1.272    1.311
    2       -0.015  -0.023  -1.272   -1.311
--------------------------------------------
tot          0.000   0.000   0.000    0.000
```

```
FREE ENERGIE OF THE ION-ELECTRON SYSTEM (eV)
---------------------------------------------------
free  energy   TOTEN  =       -15.58814939 eV
```



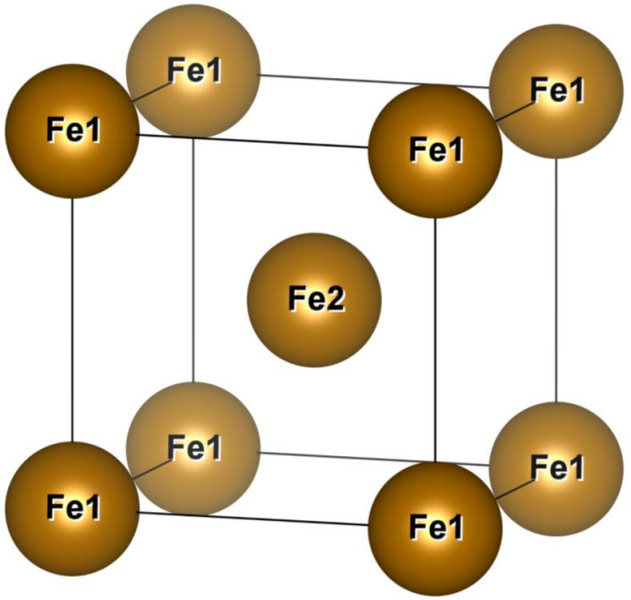
FM vs AFM

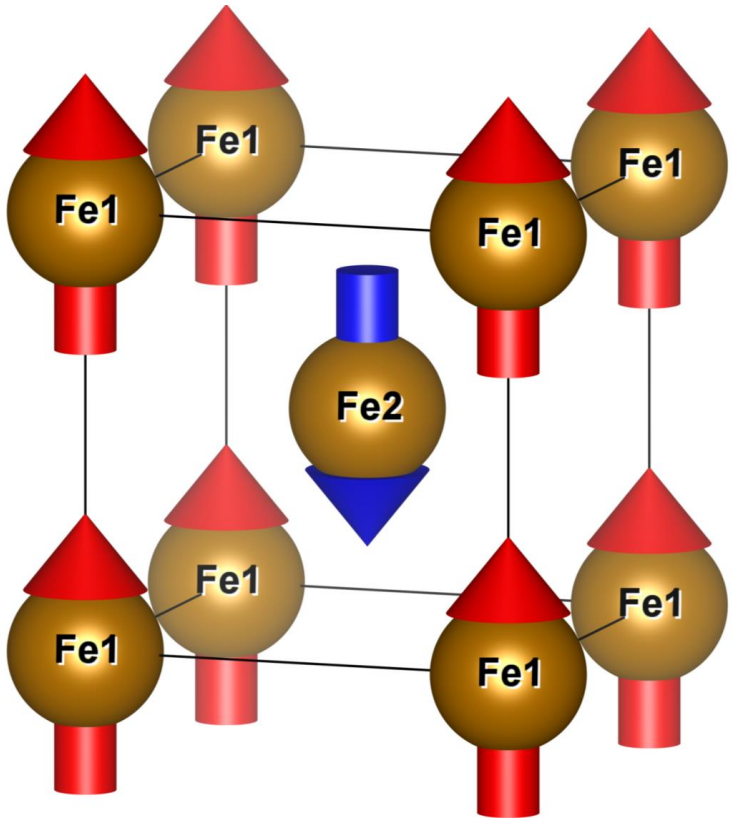
TOTEN for FM = -16.47327343 eV

TOTEN for AFM = -15.58814939 eV

More negative
More stable

FM configuration more stable than AFM configuration

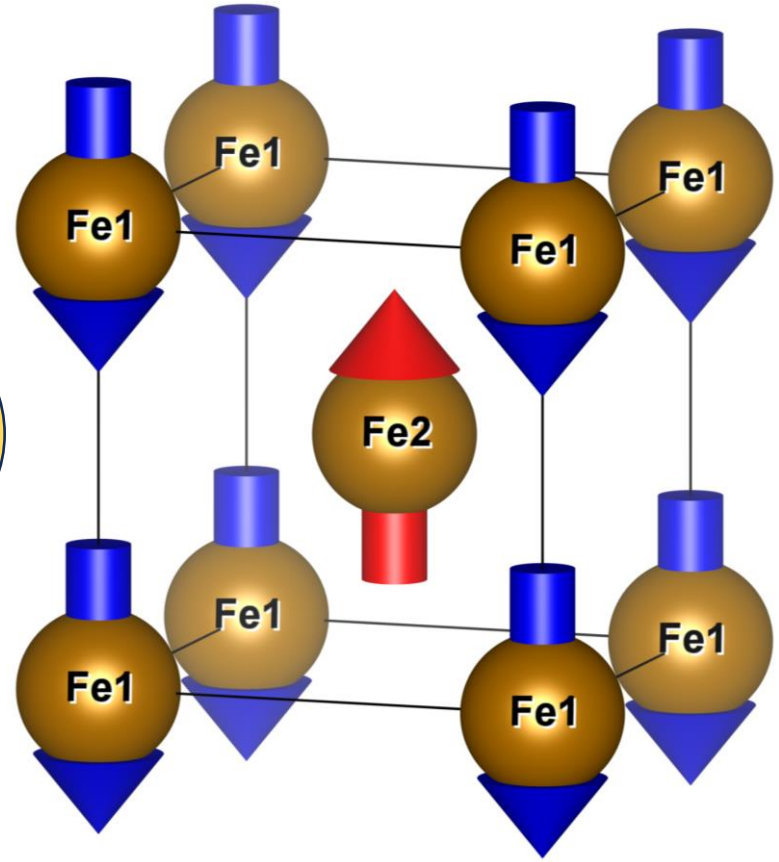




What will happen when

MAGMOM = 1*-4 1*4 ?

Same

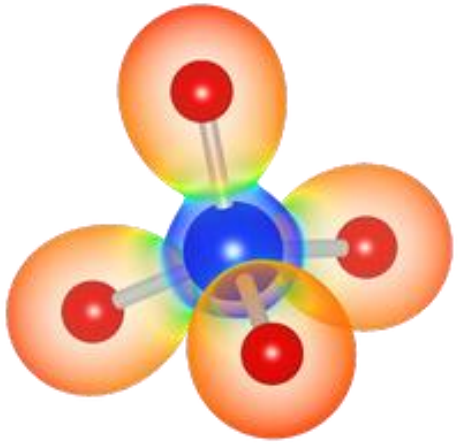


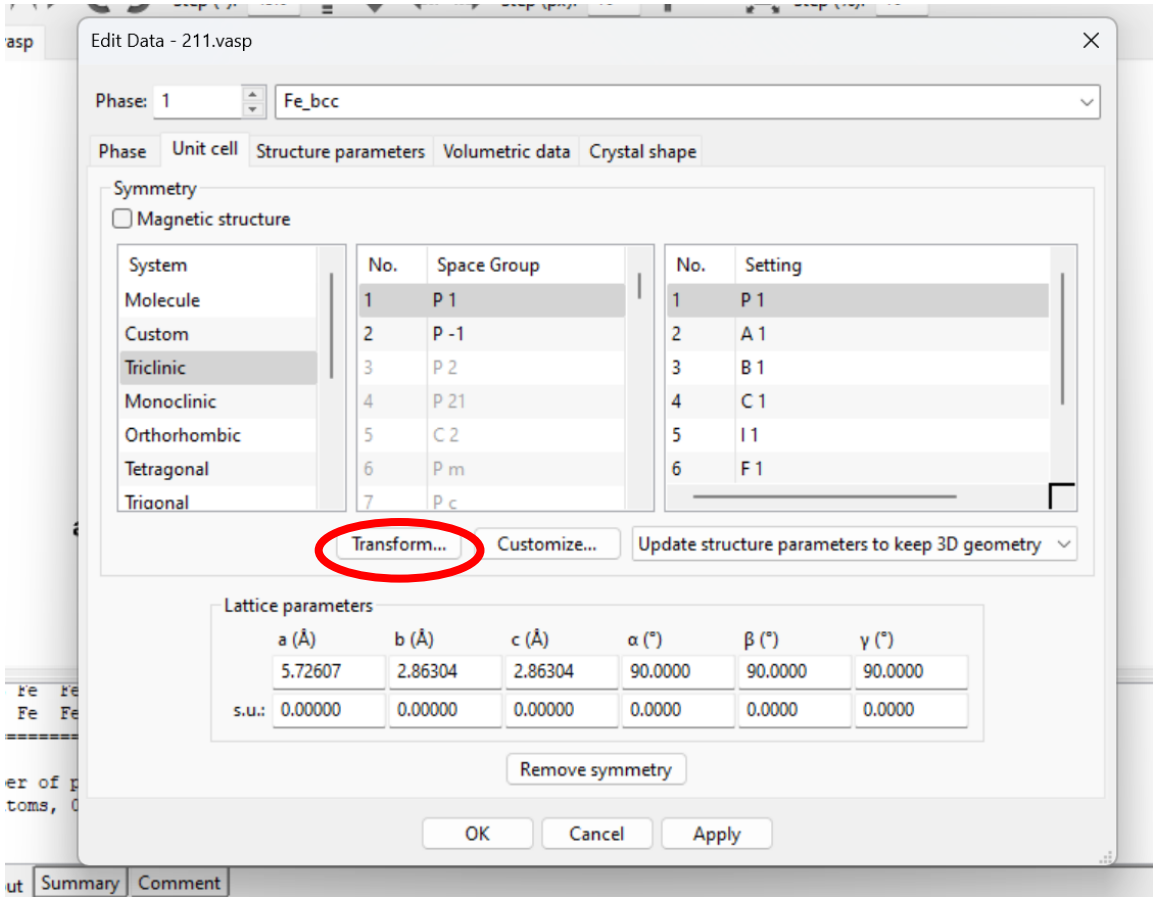
How to build AFM configuration with odd number of atoms ?

How to build AFM configuration with odd number of atoms ?

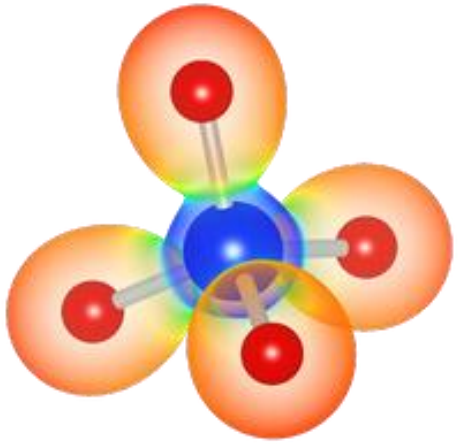
Supercell

VESTA – Supercell





VESTA – Supercell



Edit Data - 211.vasp

Phase: 1 Fe_bcc

Phase | Unit cell | Structure parameters | Volumetric data | Crystal shape

Symmetry

Magnetic structure

System: Molecule, Custom, Triclinic, Monoclinic, Orthorhombic, Tetragonal, Trigonal

No. | Space Group: 1, 2, 3, 4, 5, 6, 7

No. | Setting

Transfor

Lattice parameters

a (Å) | b (

5.72607 | 2.8

s.u.: 0.00000 | 0.0

Summary | Comment

Unit Cell Transformation

Transformation matrix

Rotation matrix (P)

1	0	0
0	1	0
0	0	1

Translation vector (p)

0.000000
0.000000
0.000000

View General Positions

Initialize current matrix

The new basis vectors a', b', c' are related to the basis vectors a, b, c by

$$(\boldsymbol{a}', \boldsymbol{b}', \boldsymbol{c}') = (\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c})\boldsymbol{P}$$

$$= (\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}) \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}$$

$$= (P_{11}\boldsymbol{a} + P_{21}\boldsymbol{b} + P_{31}\boldsymbol{c},$$
$$P_{12}\boldsymbol{a} + P_{22}\boldsymbol{b} + P_{32}\boldsymbol{c},$$
$$P_{13}\boldsymbol{a} + P_{23}\boldsymbol{b} + P_{33}\boldsymbol{c})$$

A shift of origin is defined by the shift vector

$$\boldsymbol{t} = (\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c})\boldsymbol{p}$$

$$= (\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}) \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix}$$

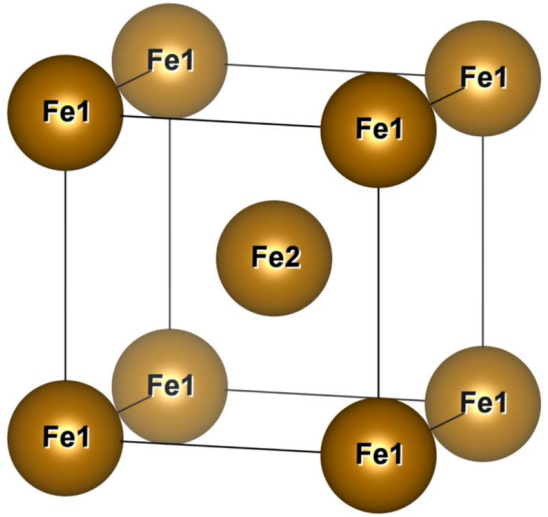
$$= p_1\boldsymbol{a} + p_2\boldsymbol{b} + p_3\boldsymbol{c}.$$

Normalize the range of fractional coordinates

OK | Cancel

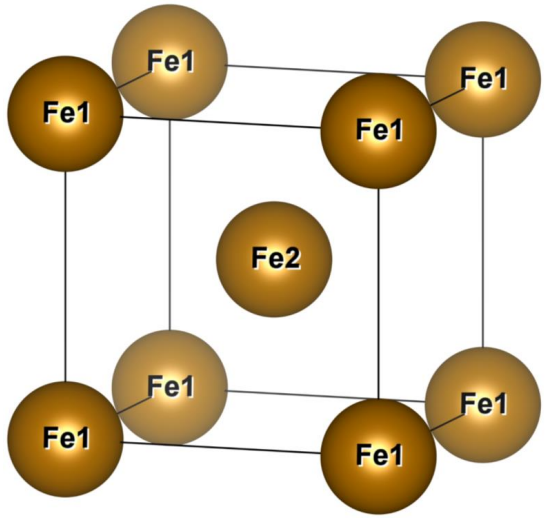
Ferrimagnetism

Can we build a ferrimagnetic structure with 2 atoms of Fe?

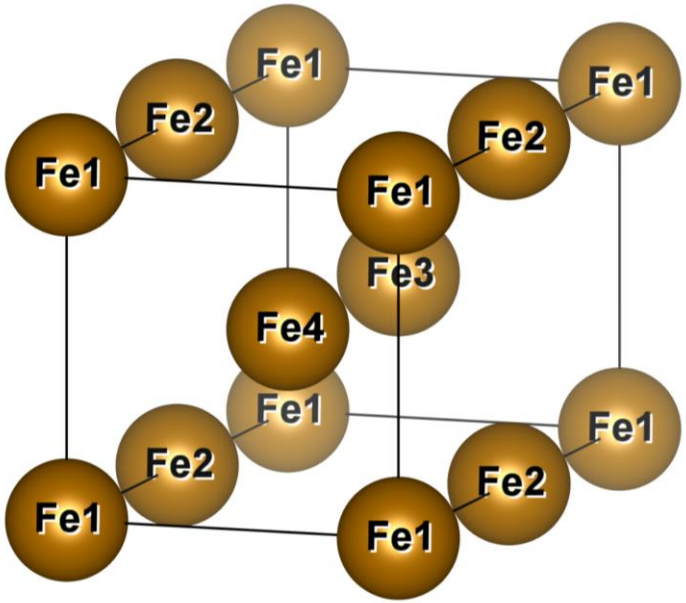


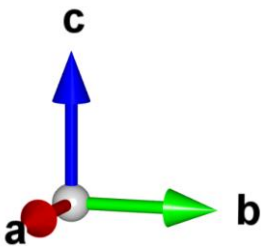
Ferrimagnetism

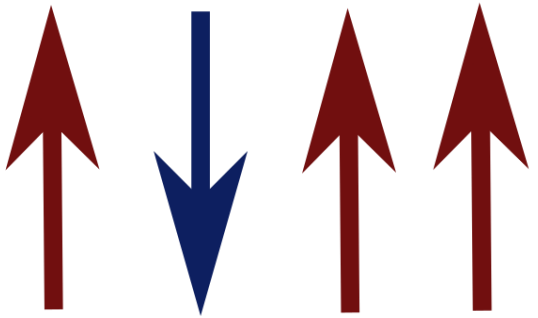
Can we build a ferrimagnetic structure with 2 atoms of Fe?



Supercell(2x1x1)



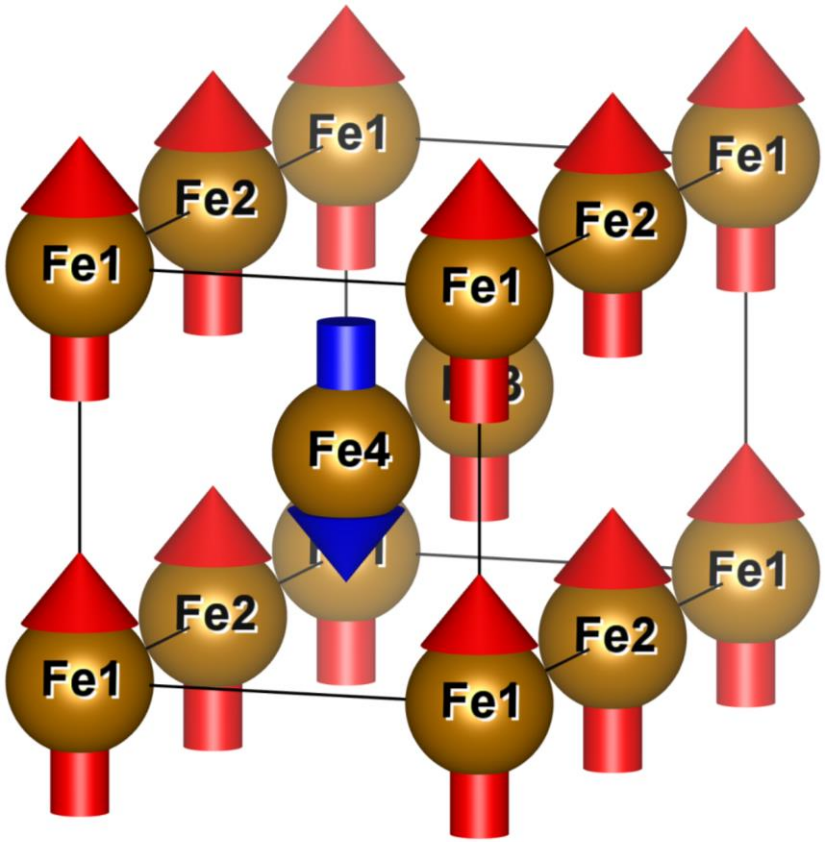




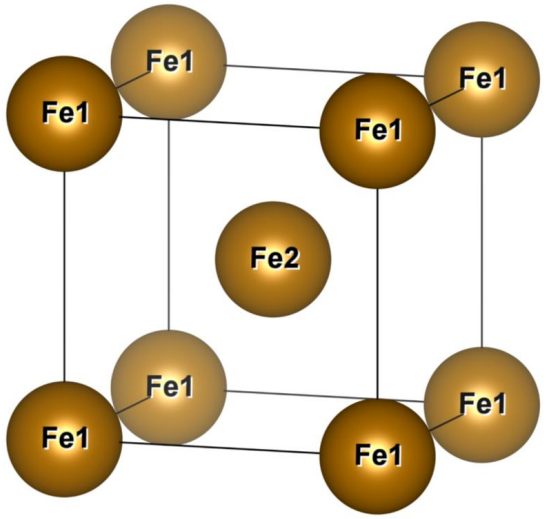
NIONS = 4

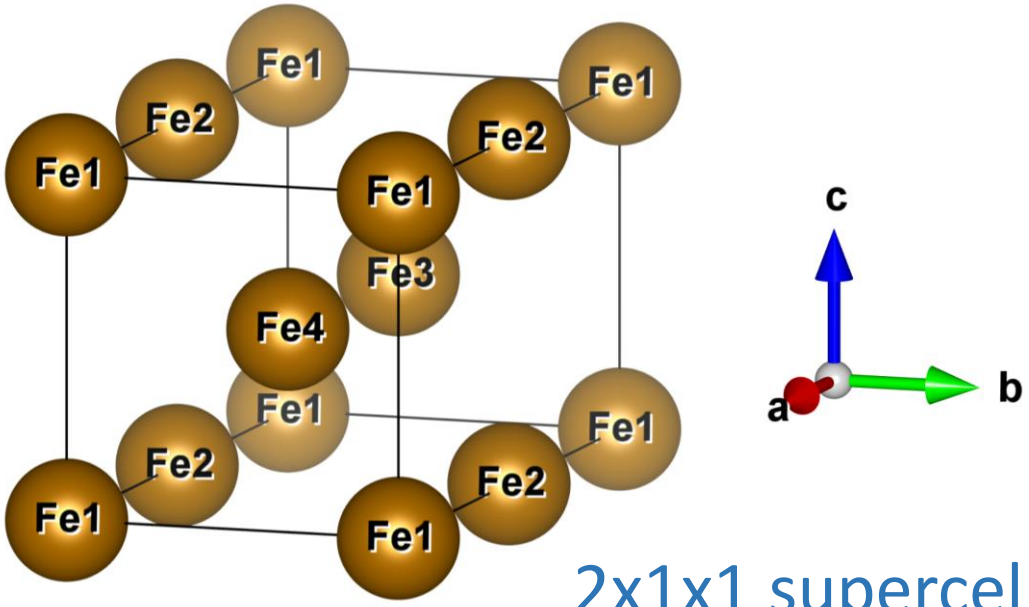
MAGMOM = 3*4 1*-4

```
ISTART=0
ISMEAR = 1
SIGMA = 0.2
ENCUT = 500
IBRION =2
NSW =300
ISIF=3
EDIFF = 0.1E-05
EDIFFG = -0.001
LORBIT = 11
PREC = Accurate
ISPIN=2
MAGMOM = 3*4 1*-4
```



What happens to KPOINTS when taking supercell?



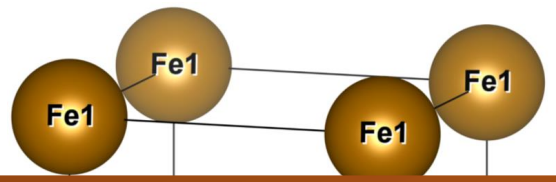


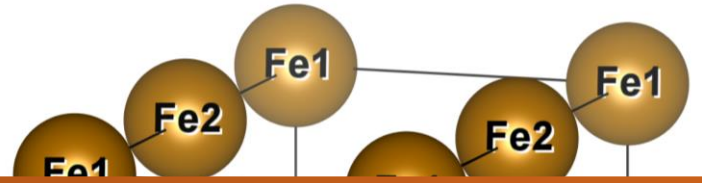
2x1x1 supercell

```
k-points
 0
Monkhorst Pack
 8 8 8
 0  0  0
```

```
k-points
 0
Monkhorst Pack
 4 8 8
 0  0  0
```

What happens to KPOINTS when taking supercell?





Computationally expensive

```
Monkhorst Pack
 8  8  8
 0  0  0
```

```
Monkhorst Pack
 4  8  8
 0  0  0
```

Magnetic Calculations

2. Calculate the magneto-crystalline anisotropy energy (MAE) of Fe by incorporating Spin-Orbit Coupling in DFT

Magnetic Anisotropy

- Strongly affects the shape of Hysteresis loop
- Can be related to the shape, stress, exchange or even can be induced — **Extrinsic**
- Crystal Anisotropy or Magnetocrystalline Anisotropy (MCA) — **Intrinsic**

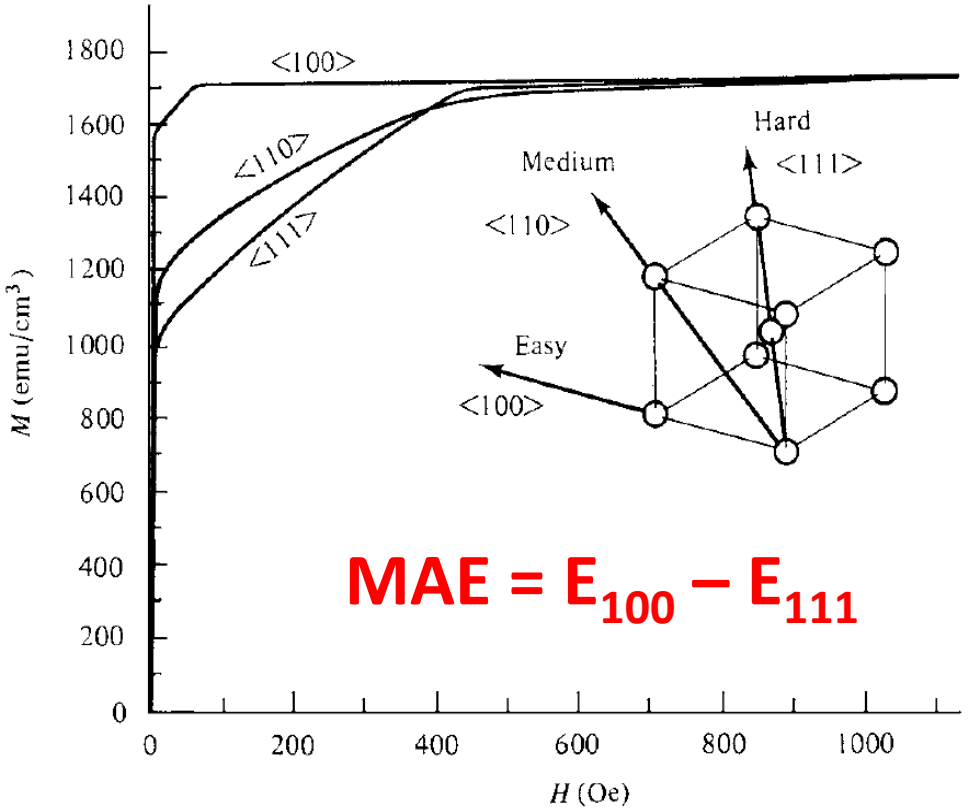
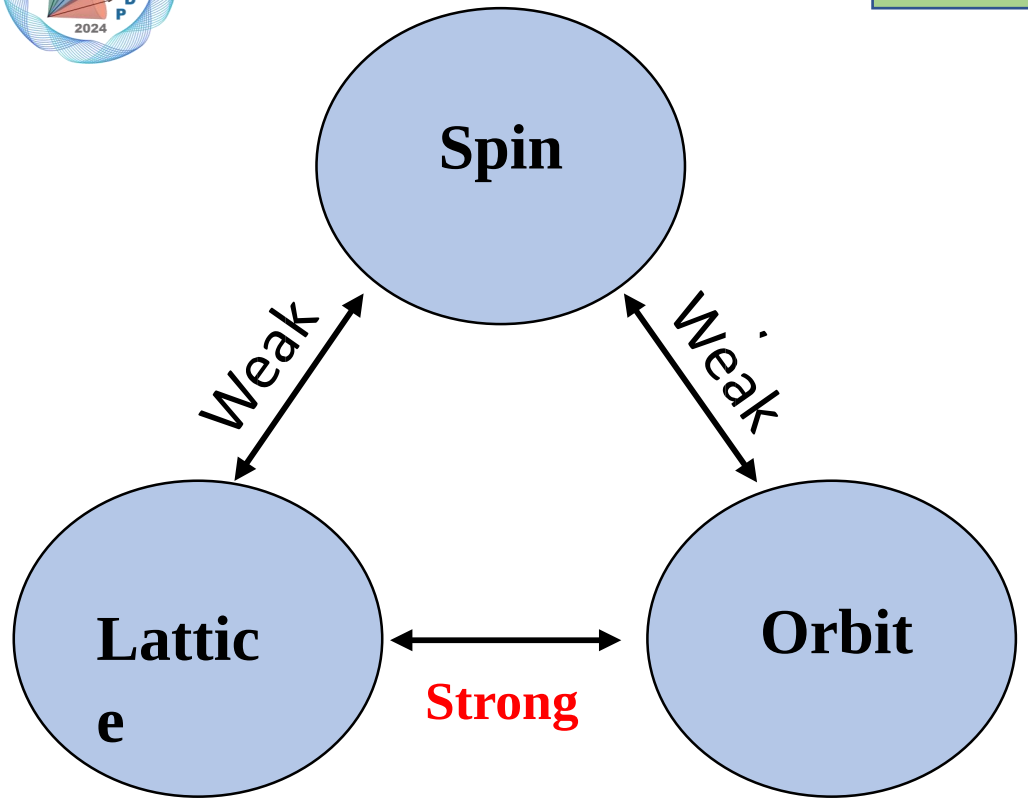


Image : BD Cullity and CD Graham, Introduction to magnetic materials

Anisotropy Constant (K) = MAE/Cell vol.

The quantity that usually distinguishes the permanent (hard) magnets from the soft ones is large anisotropy energy

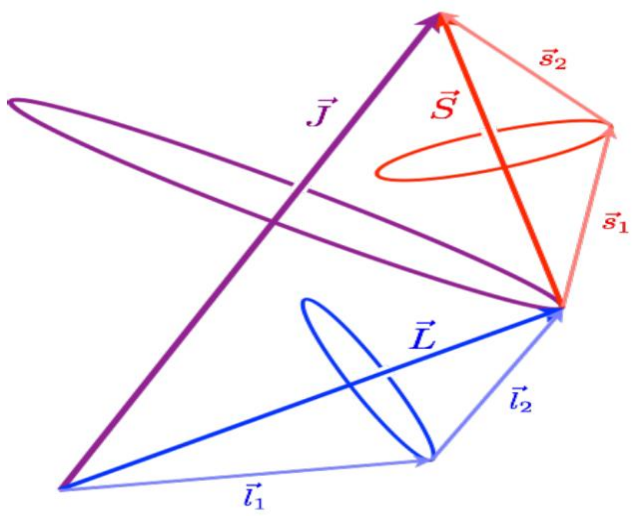
Spin-Orbit Coupling



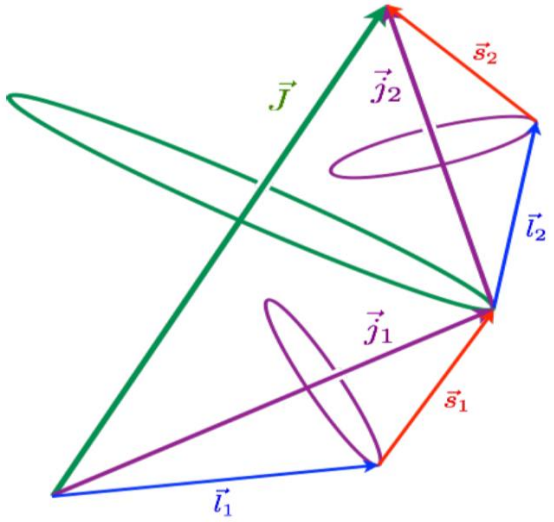
- ✓ Orbital magnetic moments are quenched to the lattice
- ✓ Spin-spin coupling is strong but is isotropic in nature
- ✓ Anisotropy energy is the energy needed to overcome spin-orbit coupling

$$E_{so} = \frac{-\mu_0 \mu_B Z^4}{4\pi a_0^3}$$

MAE is mainly due to spin-orbit coupling



LS Coupling (Lanthanides/Rare Earths)



JJ Coupling (Actinides)

Before SOC – static (point calculation/NSCF)

1. Create a new folder (mkdir static)
2. Copy CONTCAR, INCAR, POTCAR, KPOINTS and job.sh to
3. Go to static (cd static)
4. Rename CONTCAR to POSCAR (mv CONTCAR POSCAR)
5. Modify INCAR
6. Increase KPOINTS

```
k-points
 0
Monkhorst Pack
 12 12 12
 0  0  0
```

Calculation 3 :
Tut_3/Fe/static/input

```
ISTART = 0
ISMEAR = 1
SIGMA = 0.2
ENCUT = 500
IBRION = -1
NSW = 0
ISIF = 2
EDIFF = 0.1E-06
EDIFFG = -0.0001
LORBIT = 11
PREC = Accurate
ISPIN = 2
MAGMOM = 2*4
```

Magnetocrystalline anisotropy Energy (MAE)

The MAE is determined by rotating all spins according to different directions and the approach that we use is : **MAGNETIC FORCE THEOREM**

SAXIS

Page Discussion

SAXIS = [real array]

Default: **SAXIS** = (0, 0, 1)

Description: Set the global spin-quantization axis w.r.t. Cartesian coordinates.

LSORBIT = .TRUE. | .FALSE.

Default: **LSORBIT** = .FALSE.

Description: Switch on spin-orbit coupling.

For noncollinear calculation (LNONCOLLINEAR=T), the on-site magnetic moment (MAGMOM) is specified by three components for each ion.

SOC is non-collinear (ncl) – vasp_ncl in job.sh

MAGMOM = m_x m_y m_z for each atom

For BCC Fe-

MAGMOM = 0 0 2.2 0 0 2.2

Better to use the magnetic moment obtained in static run

More on Non-Collinearity

Non-collinear magnetism is quite common in nature, where the spins are not parallel (ferromagnetic) or anti-parallel (antiferromagnetic), rather they orient in spirals, helicoids, canted or disordered. Non-collinear magnetism can occur because of geometric frustration of magnetic interaction. It can also occur due to the magnetocrystalline anisotropy which is the result of interaction between the spin and lattice interaction. This relativistic effect comes via spin-orbit coupling.

density functional theory - What's the difference between spin-unpolarized, spin-polarized and non-colinear calculation? - Matter Modeling Stack Exchange

Sample INCAR for SOC calculation

```
ISTART=0
ICHARG = 11
ISMEAR = 1
SIGMA = 0.2
ENCUT = 500
ISPIN=2
MAGMOM = 0 0 2.2 0 0 2.2
SAXIS= 1 0 0
EDIFF = 1E-06
LORBIT = 11
LSORBIT = .True.
LWAVE = .False.
LCHARG= .False.
LORBMOM = T
LNONCOLLINEAR = .TRUE.
LMAXMIX = 4
ISYM = 0
PREC = Accurate
NPAR = 4
NBANDS = 32
GGA_COMPAT=.FALSE.
```

CHGCAR goes as input file

2*SCF (grep NBANDS OUTCAR)

INPUT files for SOC calculation :

INCAR
POSCAR (static CONTCAR to POSCAR)
POTCAR
KPOINTS
CHGCAR
job.sh

- Make folder SOC – mkdir SOC
- Copy all input files to SOC folder

job.sh for SOC calculation

```
#!/bin/bash
#PBS -N soc_x
#PBS -q little
#PBS -l nodes=1:ppn=4
#PBS -V

cd $PBS_O_WORKDIR

mpirun -n 4 -N 4 /home/amrb/vasp/vasp.6.2.0/bin/vasp_ncl > vasp.out
```

Magnetocrystalline anisotropy Energy (MAE)

First Method

SAXIS fixed, Change MAGMOM

1. Inside SOC folder make folder magmom_change – mkdir magmom_change
2. cd magmom_change
3. mkdir x
4. mkdir y
5. mkdir z

MAGMOM applied along 3 different directions

SAXIS = 0 0 1 (z-axis)
MAGMOM = m 0 0 m 0 0

In most cases, the changes in energies are very low (sometimes around micro-eV)

```
ISTART=0
ISMEAR = 1
SIGMA = 0.2
ENCUT = 500
ISPIN=2
MAGMOM = 2.2 0 0 2.2 0 0
SAXIS= 0 0 1
EDIFF = 1E-05
LORBIT = 11
LSORBIT = .True.
LWAVE = .False.
LCHARG= .False.
LORBMOM = T
LNONCOLLINEAR = .TRUE.
LMAXMIX = 4
ISYM = 0
PREC = Accurate
NPAR = 4
NBANDS = 32
GGA_COMPAT=.FALSE.
```

First Method : SAXIS fixed, Change MAGMOM

```
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```

```
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ISPIN=2
MAGMOM = 0 0 2.2 0 0 2.2
SAXIS= 0 0 1
EDIFF = 1E-05
LORBIT = 11
LSORBIT = .True.
LWAVE = .False.
LCHARG= .False.
LORBMOM = T
LNONCOLLINEAR = .TRUE.
LMAXMIX = 4
ISYM = 0
PREC = Accurate
NPAR = 4
NBANDS = 32
GGA_COMPAT=.FALSE.
```

First Method : SAXIS fixed, MAGMOM in X-direction

```
ISTART=0
ISMEAR = 1
SIGMA = 0.2
ENCUT = 500
ISPIN=2
MAGMOM = 2.2 0 0 2.2 0 0
SAXIS= 0 0 1
EDIFF = 1E-05
LORBIT = 11
LSORBIT = .True.
LWAVE = .False.
LCHARG= .False.
LORBMOM = T
LNONCOLLINEAR = .TRUE.
LMAXMIX = 4
ISYM = 0
PREC = Accurate
NPAR = 4
NBANDS = 32
GGA_COMPAT=.FALSE.
```

magnetization (x)

# of ion	s	p	d	tot
1	-0.011	-0.047	2.257	2.200
2	-0.011	-0.047	2.257	2.200
tot	-0.023	-0.093	4.515	4.399

magnetization (y)

# of ion	s	p	d	tot
1	-0.000	-0.000	-0.000	-0.000
2	0.000	0.000	-0.000	-0.000
tot	0.000	-0.000	-0.000	-0.000

magnetization (z)

# of ion	s	p	d	tot
1	-0.000	-0.000	0.000	0.000
2	-0.000	-0.000	0.000	0.000
tot	-0.000	-0.000	0.001	0.001

orbital moment (x)

# of ion	p	d	tot
1	0.000	0.048	0.048
2	0.000	0.048	0.048
	0.000	0.096	0.097

orbital moment (y)

# of ion	p	d	tot
1	0.000	-0.000	-0.000
2	-0.000	0.000	0.000
	-0.000	-0.000	-0.000

orbital moment (z)

# of ion	p	d	tot
1	0.000	0.000	0.000
2	0.000	0.000	0.000
	0.000	0.000	0.000

First Method : SAXIS fixed, MAGMOM in X-direction

```
ISTART=0
ISMEAR = 1
SIGMA = 0.2
ENCUT = 500
ISPIN=2
MAGMOM = 2.2 0 0 2.2 0 0
SAXIS= 0 0 1
EDIFF = 1E-05
LORBIT = 11
LSORBIT = .True.
LWAVE = .False.
LCHARG= .False.
LORBMOM = T
LNONCOLLINEAR = .TRUE.
LMAXMIX = 4
ISYM = 0
PREC = Accurate
NPAR = 4
NBANDS = 32
GGA_COMPAT=.FALSE.
```

```
 magnetization (x)

# of ion       s       p       d       tot
------------------------------------------
    1       -0.011  -0.047   2.257   2.200
    2       -0.011  -0.047   2.257   2.200
------------------------------------------
tot         -0.023  -0.093   4.515   4.399
```

```
orbital moment (x)

# of ion     p       d       tot
------------------------------------
 1          0.000   0.048   0.048
 2          0.000   0.048   0.048
------------------------------------
            0.000   0.096   0.097
```

```
        FREE ENERGIE OF THE ION-ELECTRON SYSTEM (eV)
        ---------------------------------------------------
        free  energy   TOTEN  =       -16.48600896 eV
```

Direction	TOTEN (in eV)
x	-16.48600896

First Method : SAXIS fixed, MAGMOM in Y-direction

```
ISTART=0
ISMEAR = 1
SIGMA = 0.2
ENCUT = 500
ISPIN=2
MAGMOM = 0 2.2 0 0 2.2 0
SAXIS= 0 0 1
EDIFF = 1E-05
LORBIT = 11
LSORBIT = .True.
LWAVE = .False.
LCHARG= .False.
LORBMOM = T
LNONCOLLINEAR = .TRUE.
LMAXMIX = 4
ISYM = 0
PREC = Accurate
NPAR = 4
NBANDS = 32
GGA_COMPAT=.FALSE.
```

magnetization (x)

# of ion	s	p	d	tot
1	-0.000	-0.000	-0.000	-0.000
2	0.000	0.000	-0.000	0.000
tot	0.000	0.000	-0.000	-0.000

orbital moment (x)

# of ion	p	d	tot
1	0.000	-0.000	-0.000
2	-0.000	-0.000	-0.000
	0.000	-0.000	-0.000

magnetization (y)

# of ion	s	p	d	tot
1	-0.011	-0.047	2.257	2.200
2	-0.011	-0.047	2.257	2.200
tot	-0.023	-0.093	4.515	4.399

orbital moment (y)

# of ion	p	d	tot
1	0.000	0.048	0.048
2	0.000	0.048	0.048
	0.000	0.096	0.097

magnetization (z)

# of ion	s	p	d	tot
1	-0.000	-0.000	-0.000	-0.001
2	-0.000	-0.000	-0.000	-0.001
tot	-0.000	-0.000	-0.001	-0.001

orbital moment (z)

# of ion	p	d	tot
1	0.000	-0.000	-0.000
2	0.000	-0.000	-0.000
	0.000	-0.000	-0.000

First Method : SAXIS fixed, MAGMOM in Y-direction

```
ISTART=0
ISMEAR = 1
SIGMA = 0.2
ENCUT = 500
ISPIN=2
MAGMOM = 0 2.2 0 0 2.2 0
SAXIS= 0 0 1
EDIFF = 1E-05
LORBIT = 11
LSORBIT = .True.
LWAVE = .False.
LCHARG= .False.
LORBMOM = T
LNONCOLLINEAR = .TRUE.
LMAXMIX = 4
ISYM = 0
PREC = Accurate
NPAR = 4
NBANDS = 32
GGA_COMPAT=.FALSE.
```

magnetization (y)

# of ion	s	p	d	tot
1	-0.011	-0.047	2.257	2.200
2	-0.011	-0.047	2.257	2.200
tot	-0.023	-0.093	4.515	4.399

orbital moment (y)

# of ion	p	d	tot
1	0.000	0.048	0.048
2	0.000	0.048	0.048
	0.000	0.096	0.097

FREE ENERGIE OF THE ION-ELECTRON SYSTEM (eV)

free energy TOTEN = -16.48603316 eV

Direction	TOTEN (in eV)
x	-16.48600896
y	-16.48603316

First Method : SAXIS fixed, MAGMOM in Z-direction

```
ISTART=0
ISMEAR = 1
SIGMA = 0.2
ENCUT = 500
ISPIN=2
MAGMOM = 0 0 2.2 0 0 2.2
SAXIS= 0 0 1
EDIFF = 1E-05
LORBIT = 11
LSORBIT = .True.
LWAVE = .False.
LCHARG= .False.
LORBMOM = T
LNONCOLLINEAR = .TRUE.
LMAXMIX = 4
ISYM = 0
PREC = Accurate
NPAR = 4
NBANDS = 32
GGA_COMPAT=.FALSE.
```

magnetization (x)

# of ion	s	p	d	tot
1	-0.000	-0.000	0.000	-0.000
2	0.000	-0.000	0.000	-0.000
tot	-0.000	-0.000	0.000	-0.000

magnetization (y)

# of ion	s	p	d	tot
1	-0.000	-0.000	-0.001	-0.001
2	0.000	0.000	-0.000	-0.000
tot	-0.000	-0.000	-0.001	-0.001

magnetization (z)

# of ion	s	p	d	tot
1	-0.011	-0.047	2.257	2.200
2	-0.011	-0.047	2.257	2.200
tot	-0.023	-0.093	4.515	4.399

orbital moment (x)

# of ion	p	d	tot
1	0.000	-0.000	-0.000
2	-0.000	-0.000	-0.000
	0.000	-0.000	-0.000

orbital moment (y)

# of ion	p	d	tot
1	0.000	-0.000	-0.000
2	-0.000	-0.000	-0.000
	0.000	-0.000	-0.000

orbital moment (z)

# of ion	p	d	tot
1	0.000	0.048	0.048
2	0.000	0.048	0.048
	0.000	0.096	0.097

First Method : SAXIS fixed, MAGMOM in Z-direction

```
ISTART=0
ISMEAR = 1
SIGMA = 0.2
ENCUT = 500
ISPIN=2
MAGMOM = 0 0 2.2 0 0 2.2
SAXIS= 0 0 1
EDIFF = 1E-05
LORBIT = 11
LSORBIT = .True.
LWAVE = .False.
LCHARG= .False.
LORBMOM = T
LNONCOLLINEAR = .TRUE.
LMAXMIX = 4
ISYM = 0
PREC = Accurate
NPAR = 4
NBANDS = 32
GGA_COMPAT=.FALSE.
```

magnetization (z)

# of ion	s	p	d	tot
1	-0.011	-0.047	2.257	2.200
2	-0.011	-0.047	2.257	2.200
tot	-0.023	-0.093	4.515	4.399

orbital moment (z)

# of ion	p	d	tot
1	0.000	0.048	0.048
2	0.000	0.048	0.048
	0.000	0.096	0.097

```
FREE ENERGIE OF THE ION-ELECTRON SYSTEM (eV)
---------------------------------------------------
free  energy   TOTEN  =       -16.48602935 eV
```

Direction	TOTEN (in eV)
x	-16.48600896 (hard)
y	-16.48603316 (easy)
z	-16.48602935

Magnetocrystalline anisotropy Energy (MAE)

SAXIS fixed, Change MAGMOM

SAXIS = 0 0 1 (z-axis)

MAGMOM = m_x 0 0 m_x 0 0
MAGMOM = 0 m_y 0 0 m_y 0
MAGMOM = 0 0 m_z 0 0 m_z

SAXIS change, fix MAGMOM

MAGMOM = 0 0 m_z 0 0 m_z

SAXIS = 1 0 0
SAXIS = 0 1 0
SAXIS = 0 0 1

Thank You