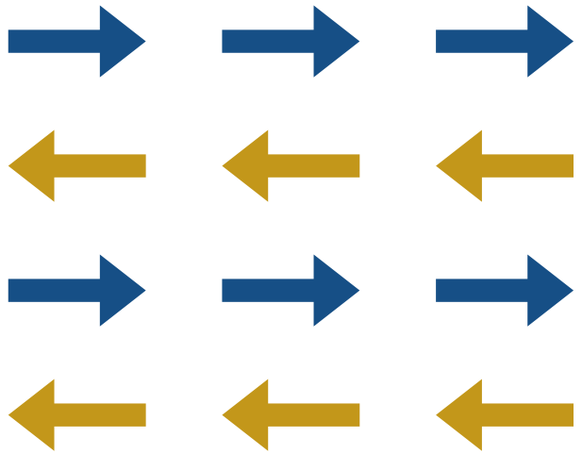
Complex crystal structures:

Anti-ferromagnets

Advanced VAMPIRE workshop

UNIVERSITY of York

Anti-ferromagnets

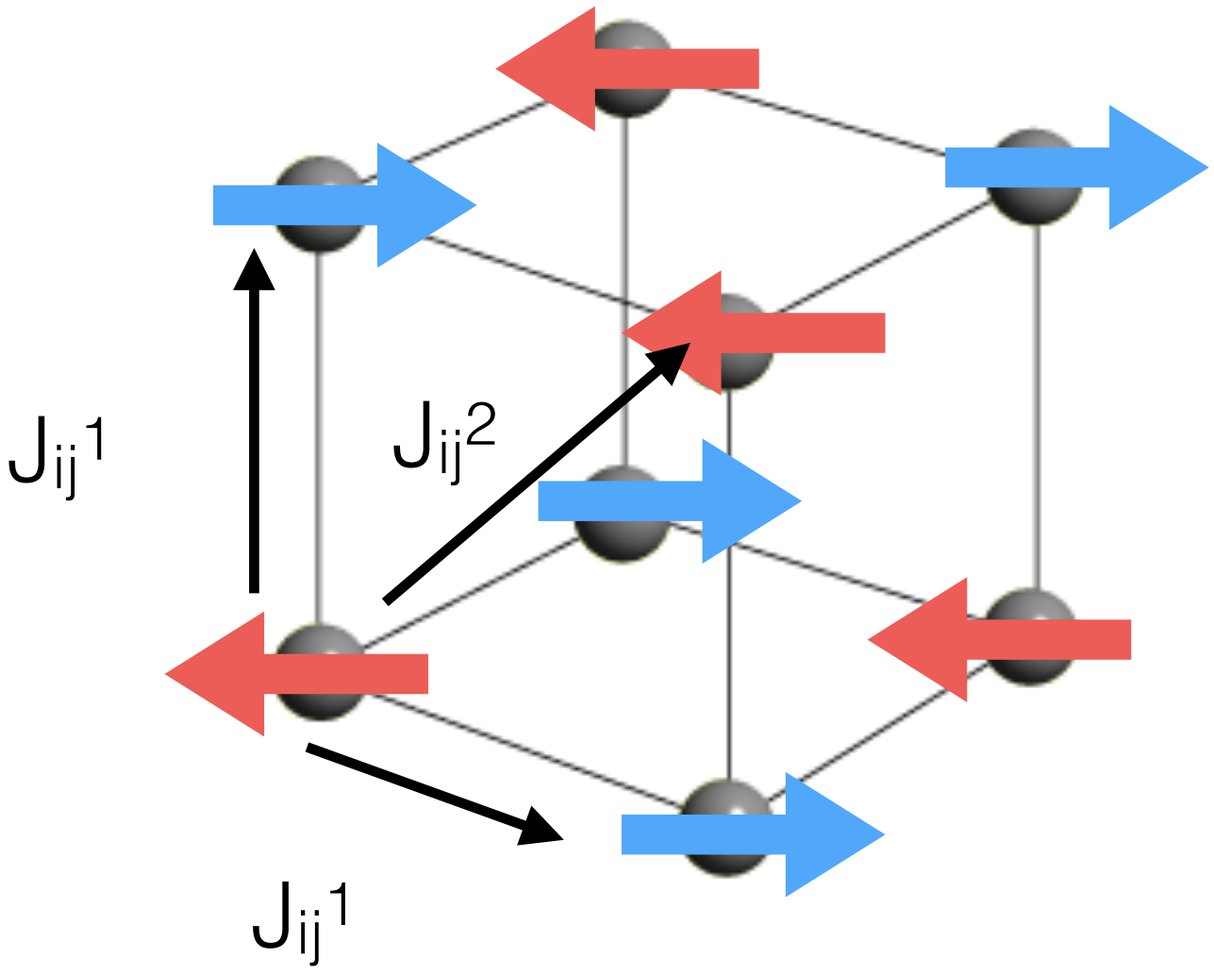


$$\mathscr{H} = -\sum_{i,j} J_{ij}\,\mathbf{S}_i \cdot \mathbf{S}_j$$

J = positive : FM
J = negative : AFM

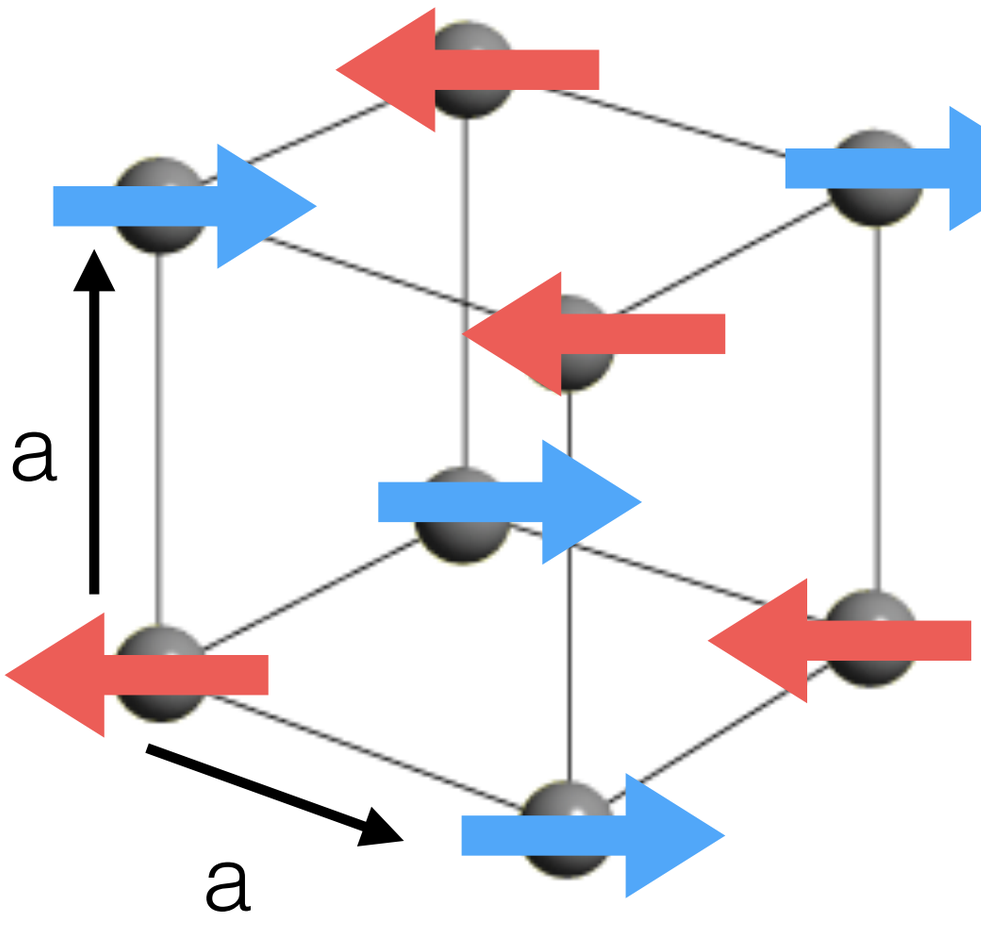
- Are technologically important materials. Due to exchange bias and anti-ferromagnetic spintronics.
- The bulk magnetisation of an AFM is 0, therefore micro magnetic modelling is too simple to model the complex physics involved.

A simple AFM



- Simple cubic structure.
- Two sub lattices - 2 materials in the unit cell
- Planes of anti-parallel magentisation.
- The $J_{ij}^{1\,(NN)}$ exchange is anti-ferromagnetic. Between atoms in different sub lattices.
- The $J_{ij}^{2(NNN)}$ is ferromagnetic. Between atoms in the same sub lattice is FM.

The unit cell



- What is the minimum repeatable magnetic and crystallographic structure?

- In this case the unit cell contains 4 atom from each sublattice. So the unit cell contains 8 atoms.

Format for the unit cell file

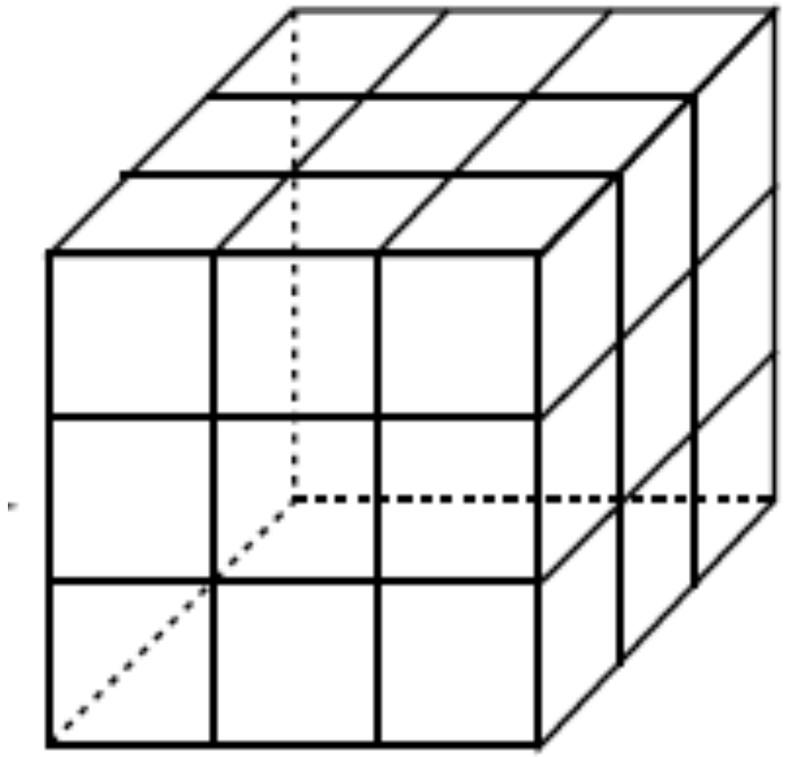
#unit cell size
2*a 2*a 2*a
#unit cell vectors
1 0 0
0 1 0
0 0 1
#Atoms
number of atoms. number of materials

atom id	**x**	**y**	**z**	**material**	**height**	**width**
0 -8				(sublattice)	0	0

The interaction list

- Interactions don't only occur within the unit cell. Each atom will also interact with atoms outside the unit cell.

- Create 26 unit cells, surrounding your initial unit cell.

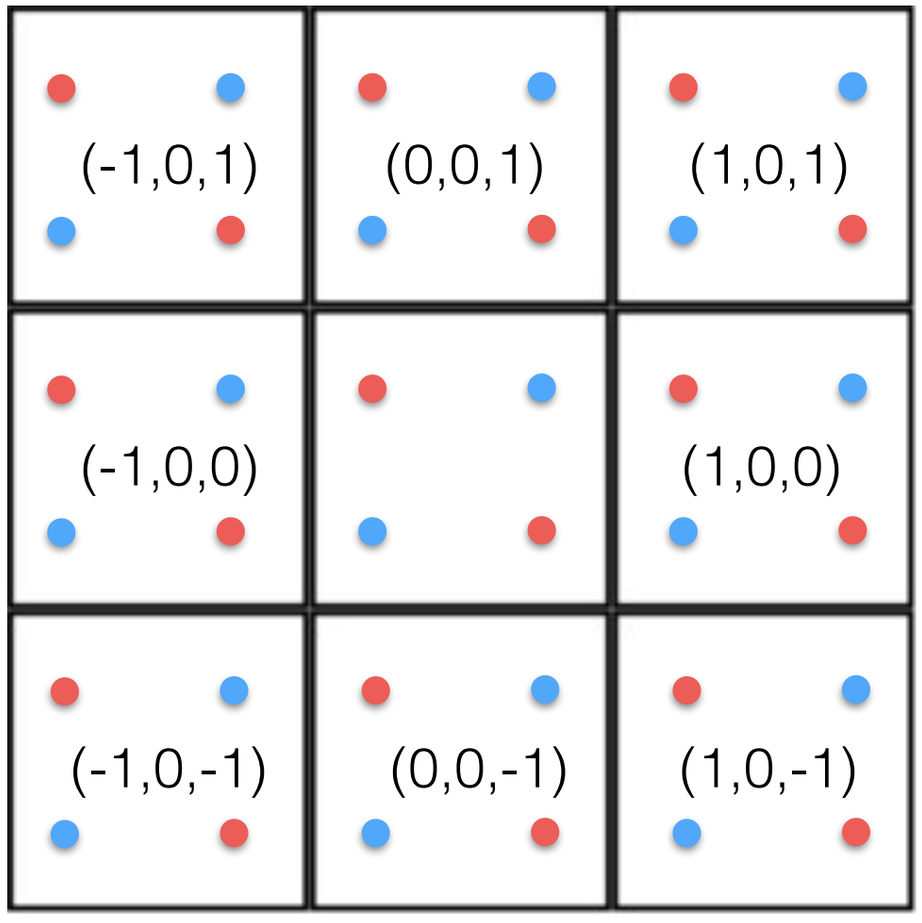


- 6 NN interactions

- 12 NNN interactions

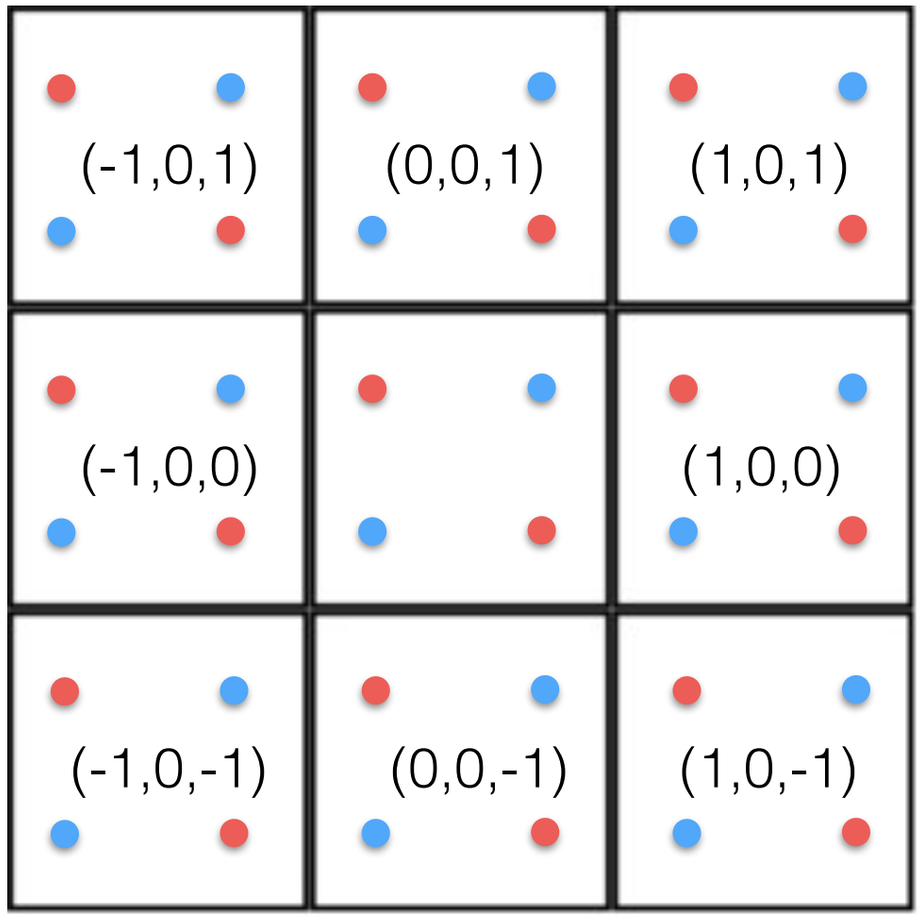
The interaction list

- Calculate which atoms are nearest neighbours and which are next nearest neighbours with the atoms in the initial unit cell.
- Loop over atoms in the initial cell (atom i).
- Loop over all the other atoms (atom j).
- Calculate the distance between atoms i and j.
- Are they nearest neighbours, next nearest neighbours or neither?



The interaction list

- If they are neighbours add to a list.
- Store dx,dy,dz and the atom id of both atoms to an array.



Creating the unit cell file

How many interactions should there be?
Check the number of interactions is equal to your prediction.

#interactions
number of interactions. “normalised-isotropic”

Interaction id	atom i - atom id	atom j - atom id	dx	dy	dz	interaction strength
0 - N N = (18*8)	0 -7	0 -7	-1 or 0 or1	-1 or 0 or1	-1 or 0 or1	1

Material parameters

```
material:num-materials=2

material[1]:material-name="Mn"
material[1]:damping-constant=1.0
material[1]:atomic-spin-moment=2.6 !muB
material[1]:material-element="C"
material[1]:density = 1.00
material[1]:initial-spin-direction=random
material[1]:exchange-matrix[1] = 1.4e-21
material[1]:exchange-matrix[2] = -1.4e-21


material[2]:material-name="Mn"
material[2]:damping-constant=1.0
material[2]:atomic-spin-moment=2.6 !muB
material[2]:material-element="C"
material[2]:density = 1.00
material[2]:initial-spin-direction=random
material[2]:exchange-matrix[1] = -1.4e-21
material[2]:exchange-matrix[2] = 1.4e-21
```

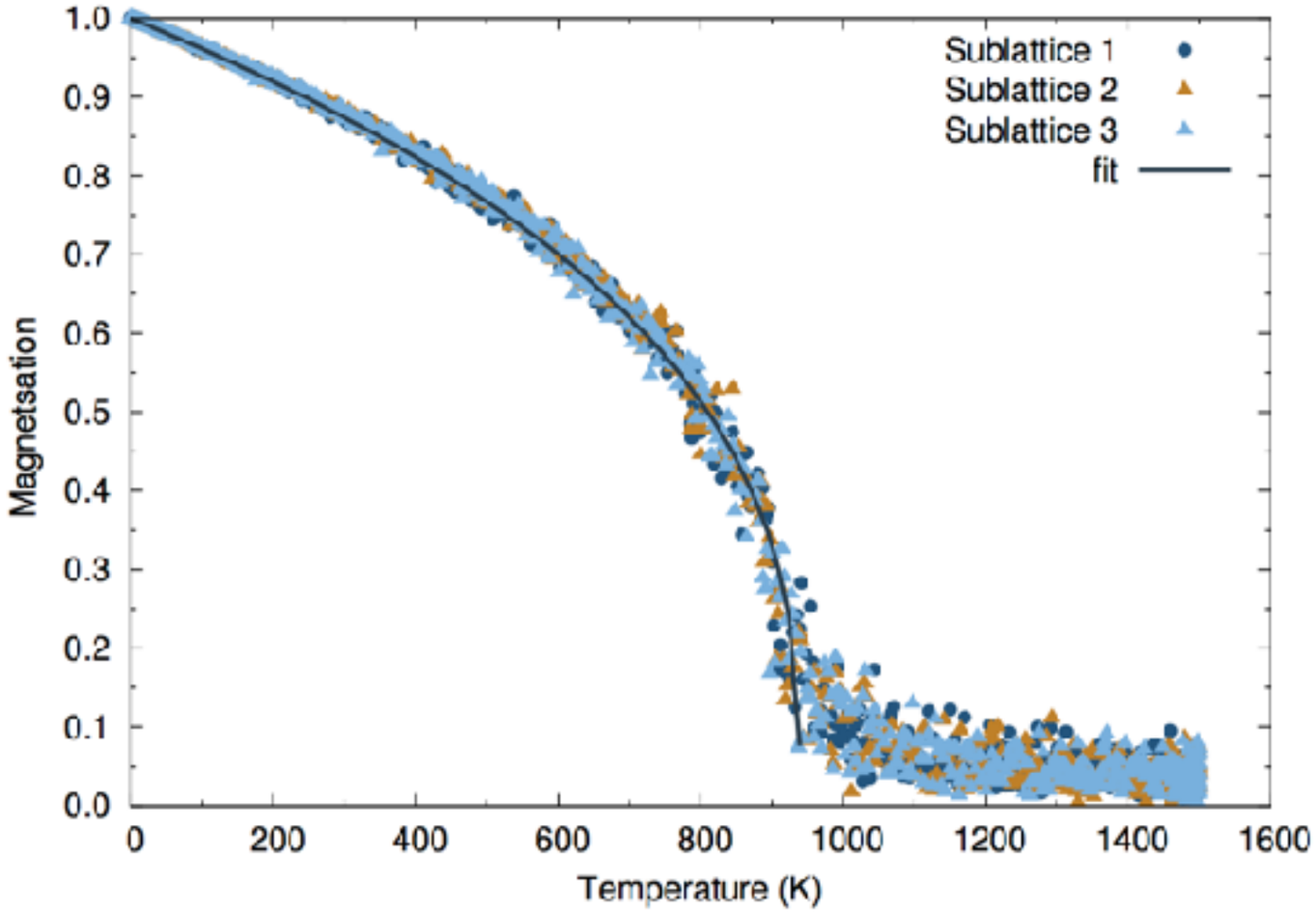
Field-cooling simulation

Neel temperature calculations

```
dimensions:system-size-x = 2 !nm
dimensions:system-size-y = 2 !nm
dimensions:system-size-z = 3 !nm


create:periodic-boundaries-x
create:periodic-boundaries-y
create:periodic-boundaries-z

material:file=AFM.mat
material:unit-cell-file= "AFM.ucf"

sim:time-step=1.0E-16
sim:time-steps-increment=1000
sim:maximum-temperature = 800
sim:minimum-temperature = 0.0
sim:cooling-function = linear
sim:cooling-time = 0.1 !ns
sim:total-time-steps = 1000000
sim:temperature = 0
```

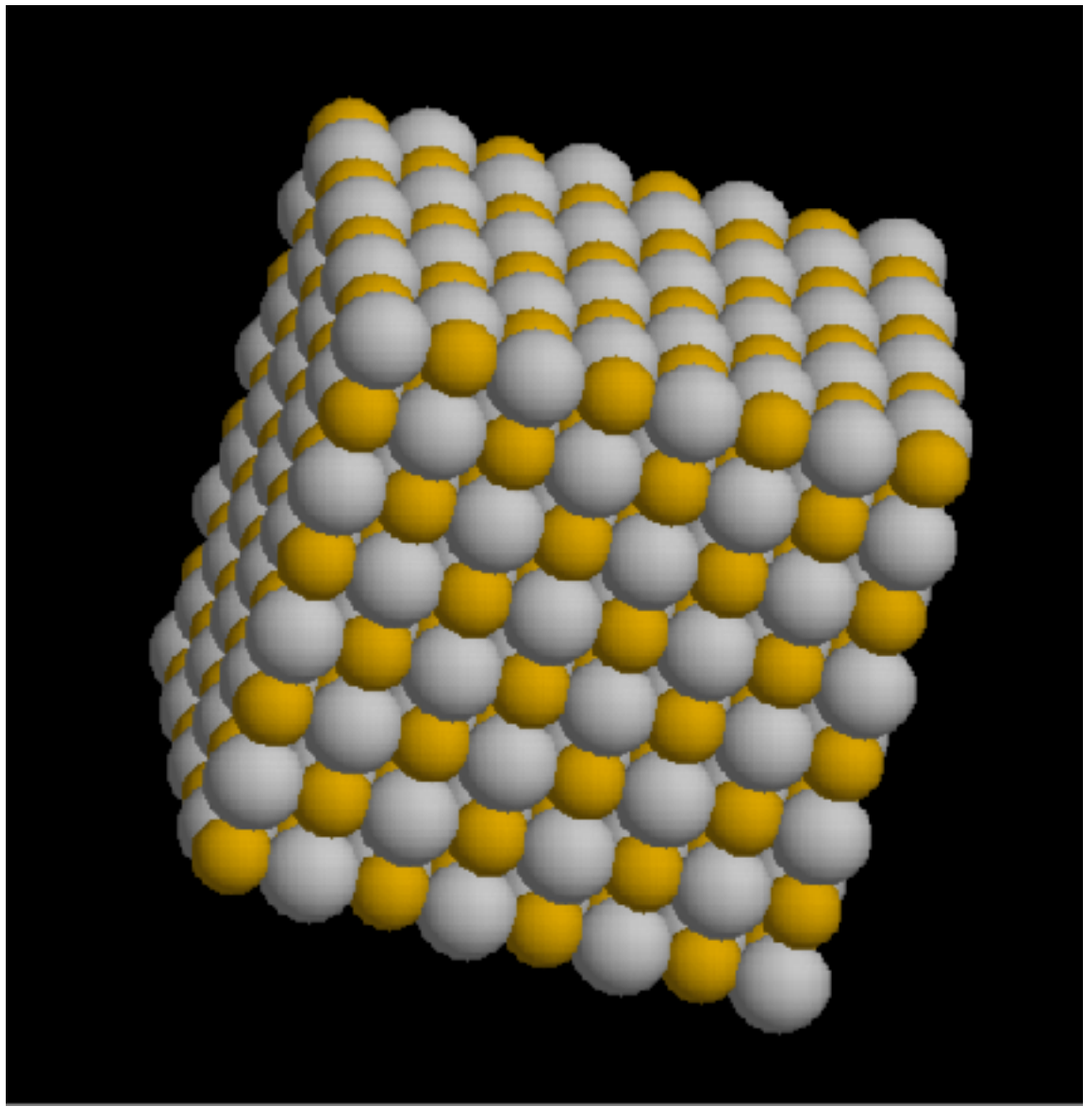
```
sim:program=field-cool
sim:integrator=llg-heun

output:real-time
output:temperature
output:material-magnetisation
screen:temperature
screen:material-magnetisation

config:atoms
config:atoms-output-rate = 1000
config:output-format = binary
```

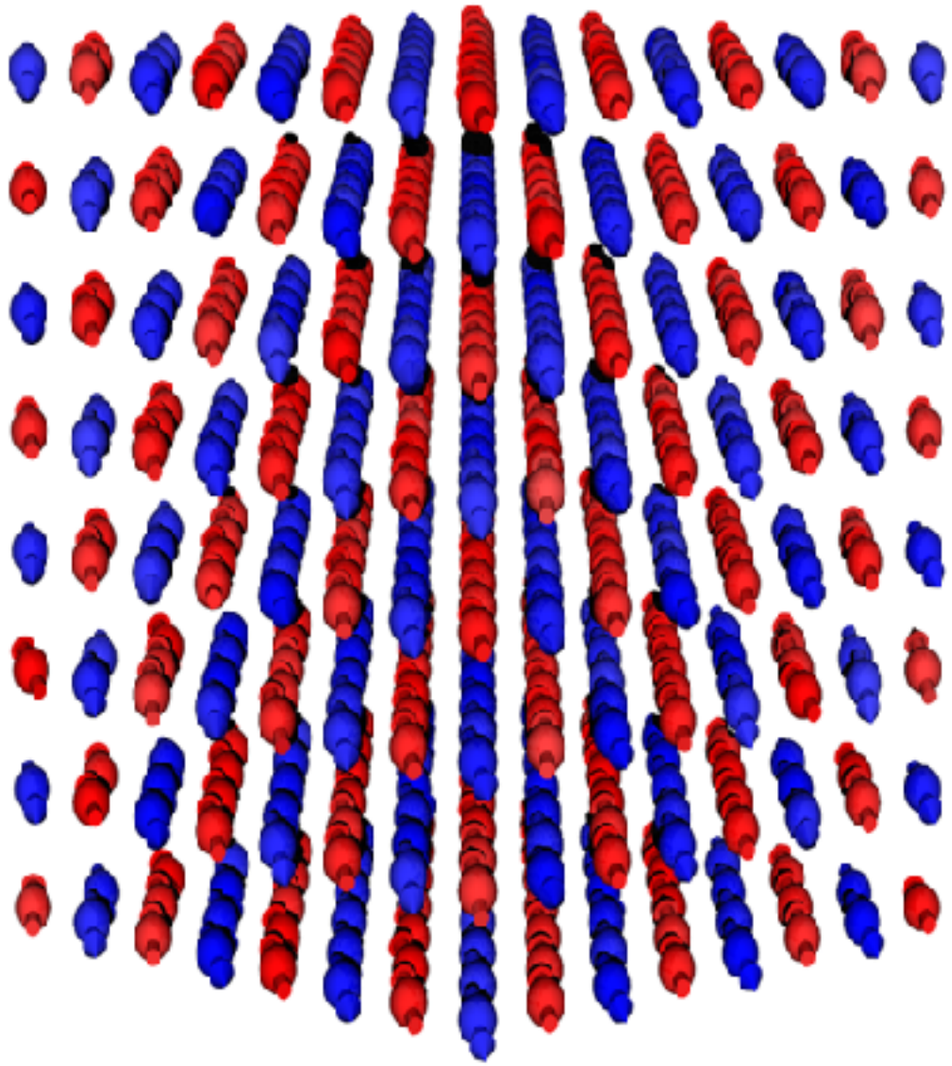
How do you calculate the magnetisation of an AFM?



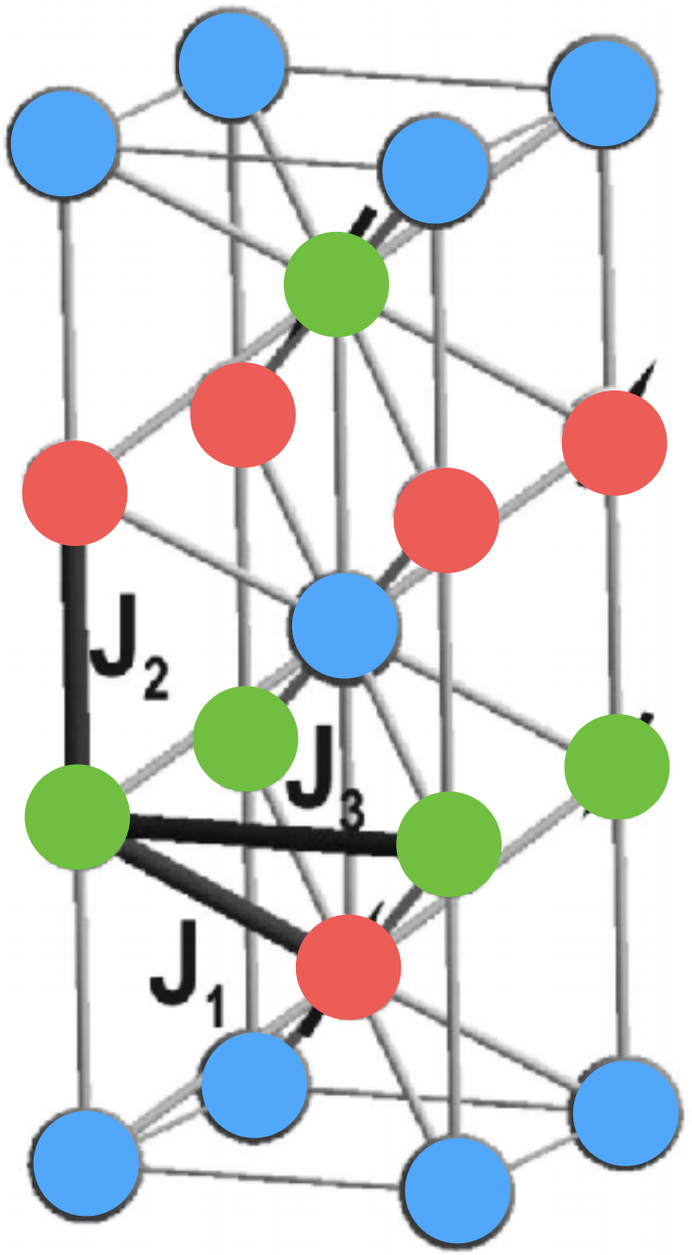
- An AFM is magnetically neutral, therefore you cant gain any information from looking at the bulk magnetisation.
- However, in each sublattice the atomic moments are aligned - giving each sublattice a high magnetisation.
- M =(m1 + m2)/2
- Then you can fit as for a normal FM.

magnetic ground state





Mn2Au - Unit Cell



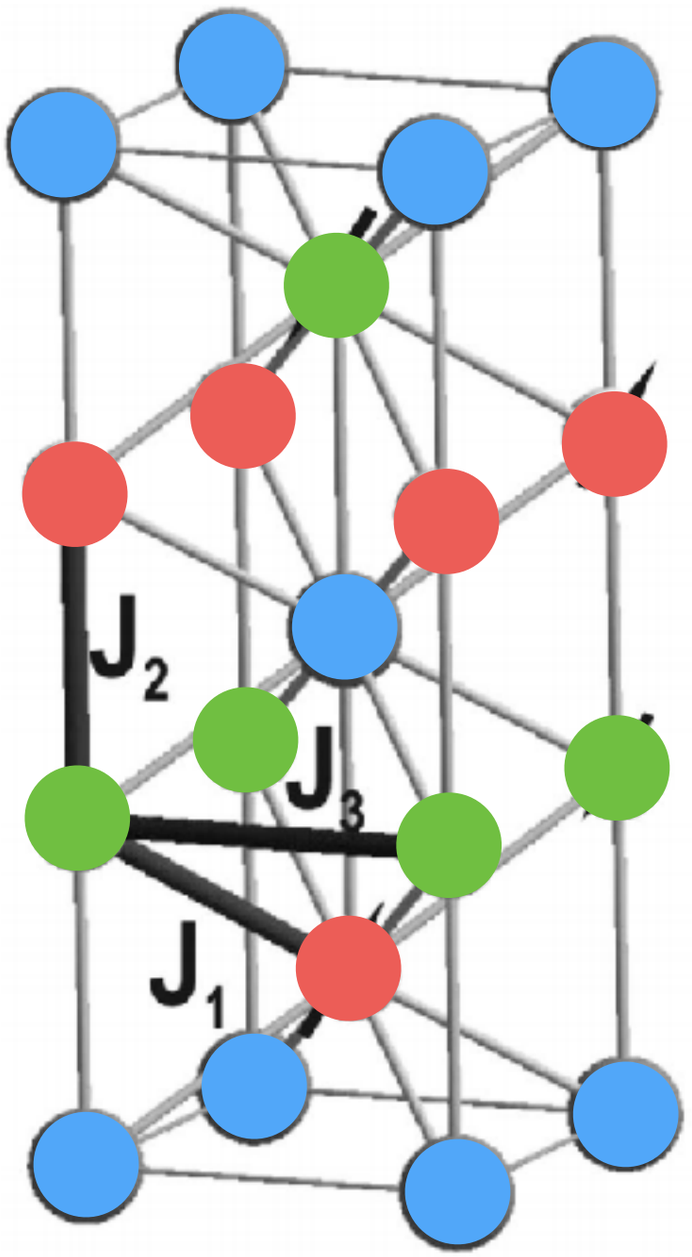
- There are 3 atoms in the unit cell. Which 3?
- Again 1 from each sublattice.
- 2 sublattices are Mn, 1 sublattice is gold.
- Create a file which outputs the 3 atoms in the unit cell. In the same format as before.

Format for the unit cell file

#unit cell size
a a c
#unit cell vectors
1 0 0
0 1 0
0 0 1
#Atoms
number of atoms. number of materials

atom id	**x**	**y**	**z**	**material**	**height**	**width**
0 -2				(sublattice)	0	0

Exchange interactions



- J1 = -10.88e-21
- J2 = -14.62e-21
- J3 = 4.18e-21
- 8 J1 interactions (4 to each other sub lattice)
- 2 J2 interactions (1 to each other sublattice)
- 4 J3 interactions (same sublattice)
- a = 3.328A c = 8.539A

Creating the unit cell file

How many interactions should there be?
Check the number of interactions is equal to your prediction.
Repeat the procedure for repeating the unit cell 27 times and finding the interactions.

#interactions
number of interactions. “normalised-isotropic”

Interaction id	atom i - atom id	atom j - atom id	dx	dy	dz	interaction strength
0 - N	0,1	0,1	-1,0,1	-1,0,1	-1,0,1	0-1

Material file

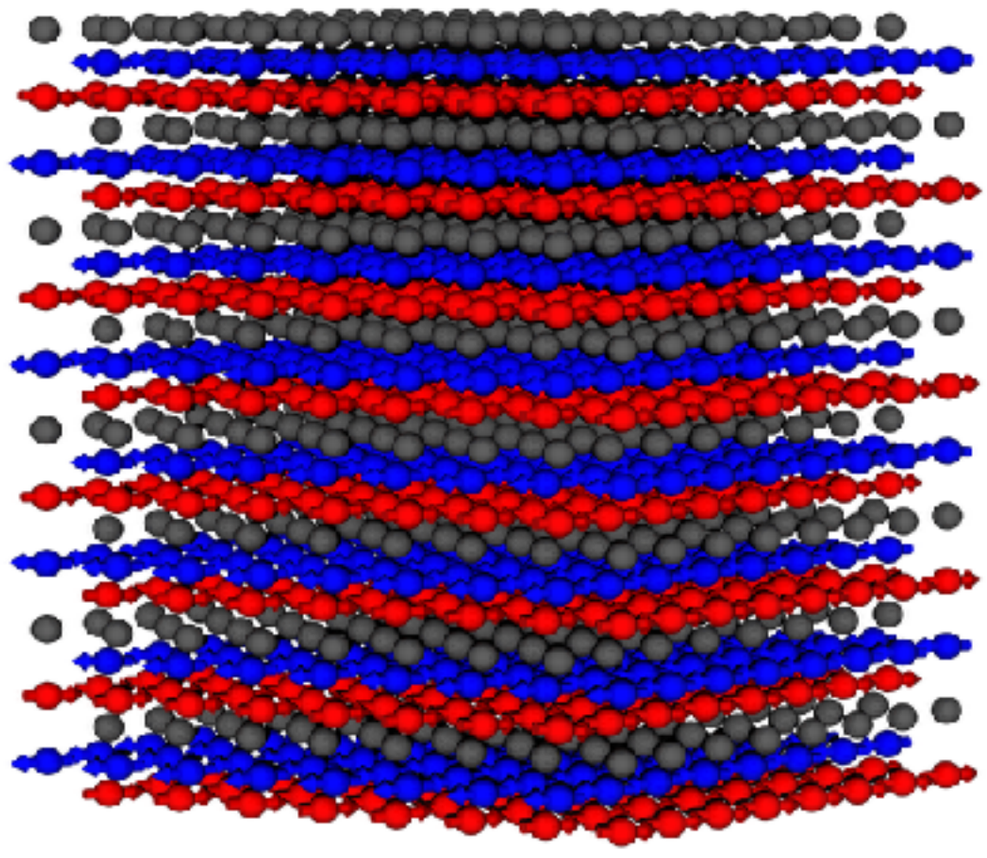
```
material[1]:material-name="Mn"
material[1]:damping-constant=1.0
material[1]:atomic-spin-moment=3.79 !muB
material[1]:material-element="C"
material[1]:density = 1.00
material[1]:initial-spin-direction=random
material[1]:exchange-matrix[1] = 6.67 !mRyd
material[1]:exchange-matrix[2] = 6.67 !mRyd
material[1]:uniaxial-anisotropy-constant=-9e-24

material[2]:material-name="Mn"
material[2]:damping-constant=1.0
material[2]:atomic-spin-moment=3.79 !muB
material[2]:material-element="Mn"
material[2]:density = 1.00
material[2]:initial-spin-direction=random
material[2]:exchange-matrix[1] = 6.67 !mRyd
material[2]:exchange-matrix[2] = 6.67 !mRyd
material[2]:uniaxial-anisotropy-constant=-9e-24

material[3]:material-name="Au"
material[3]:non-magnetic
```

- weak uniaxial anisotropy.
- strong exchange
- Au is non magnetic.

Neel temperature

- The Néel temperature of Mn2Au is approximately 1300K.

- The anisotropy means the atoms lie in plane in alternating anti-parallel layers.



Iridium Manganese - the unit cell

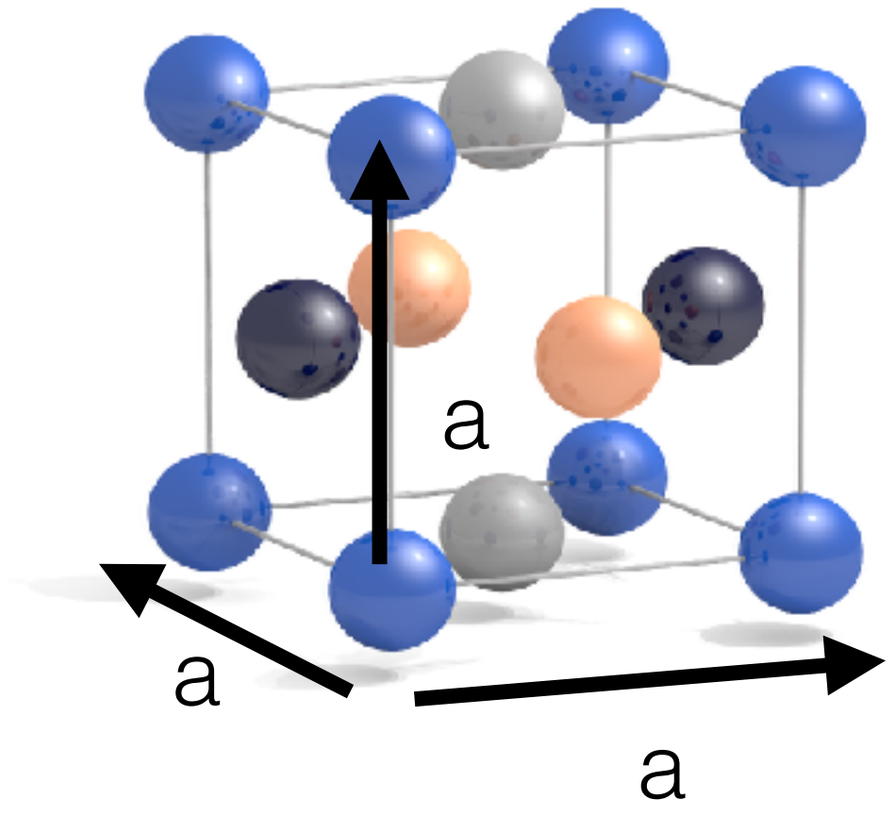
- IrMn has a FCC structure with a unit cell constant of a = 3.75 A

- Therefore, information about the crystal structure and magnetic properties can be gained by looking at the individual sub lattice magnetisations.

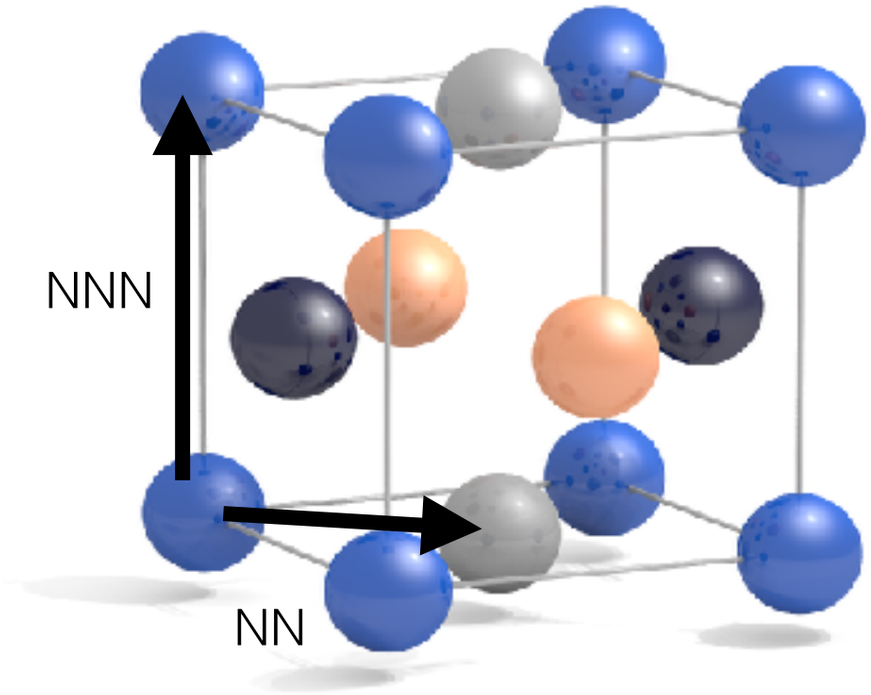
- Iridium Manganese has 4 sublattices.

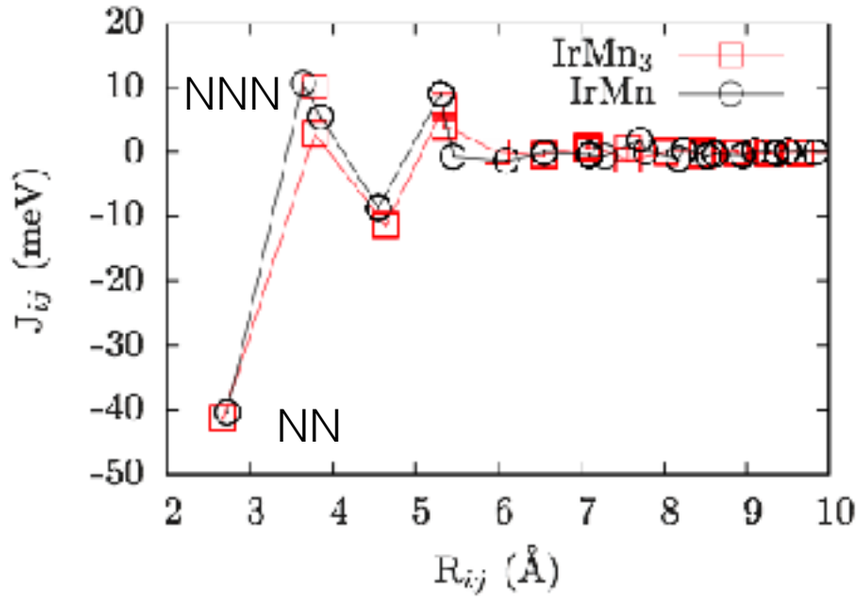
- The unit cell comprises one atom from each sublattice and is the minimum repeating magnetic and crystallographic structure.

- The spin moment of Mn =



The Exchange Constants

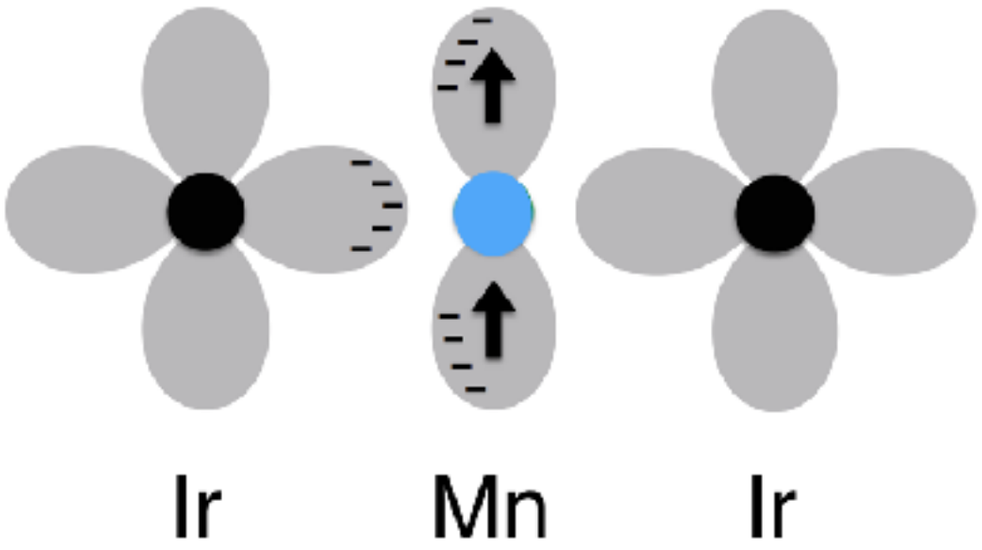




- nearest neighbour (NN) interactions occur between atoms of neighbouring sublattices.
- next nearest neighbour interactions occur between atoms of the same sublattice.
- $J_{ij}^{NN} = -6.4 \times 10^{-21}$ J/link
- $J_{ij}^{NNN} = 5.1 \times 10^{-21}$ J/link
- Therefore atoms in the same sublattices align and other sub lattices try and align 180 degrees apart.

L., Szunyogh Physical Review B **79** (2009)

The anisotropy



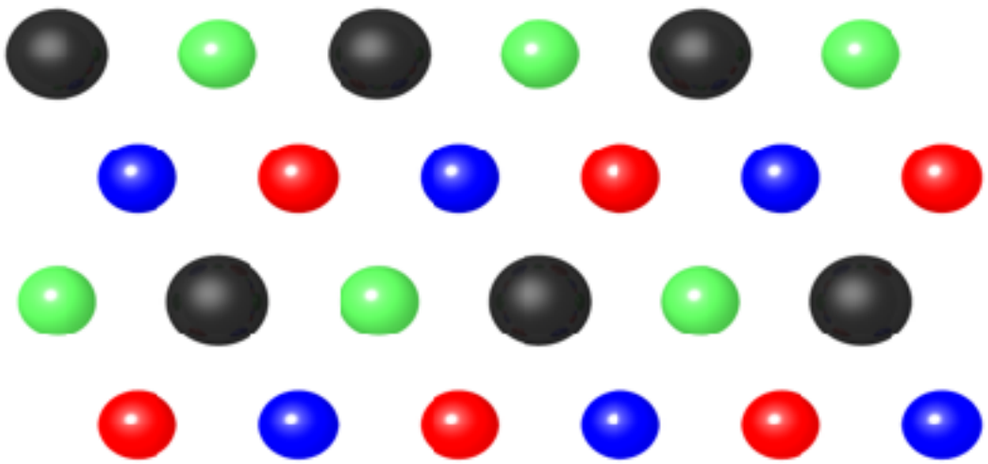
$$\mathscr{H} = -\sum_{i,j} \frac{k_{\mathrm{N}}}{2} (\mathbf{S}_i \cdot \mathbf{e}_{ij})^2$$

- Iridium atoms have large orbitals and Mn atoms have none spherical orbitals.
- The moment of the Mn atoms is repelled from the larger Ir orbitals.
- This is modelled using the Néel surface anisotropy model.
- $k_n = 4.22 \times 10^{-22}$

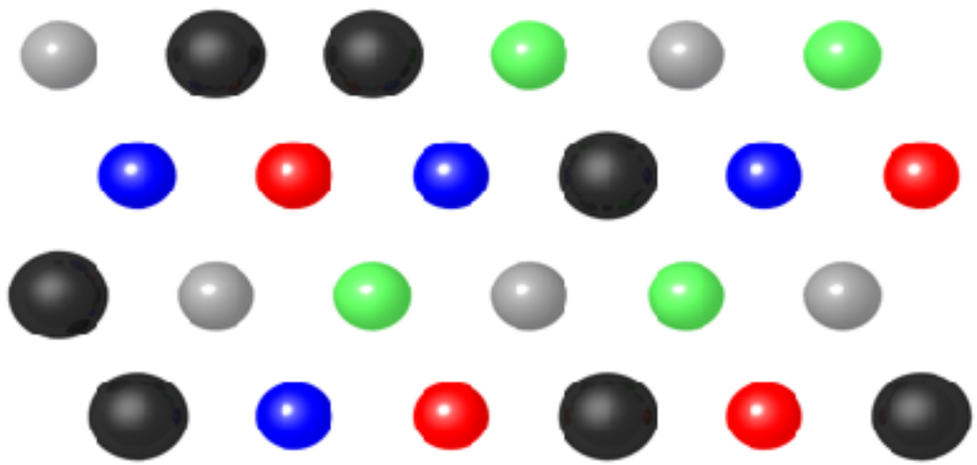
Composition

```
material[1]:material-name="Mn"
material[1]:damping-constant=1.0
material[1]:atomic-spin-moment=2.6 !muB
material[1]:surface-anisotropy-constant[5]=-4.22e-22
material[1]:material-element="C"
material[1]:density = 1.00
material[1]:initial-spin-direction=random
material[1]:exchange-matrix[1] = 6.4e-21
material[1]:exchange-matrix[2] = 6.4e-21
material[1]:exchange-matrix[3] = 6.4e-21
material[1]:exchange-matrix[4] = 6.4e-21
material[1]:host-alloy
material[1]:alloy-fraction[5]=0.25


material[5]:material-name="Ir"
material[5]:non-magnetic=keep
```

Order

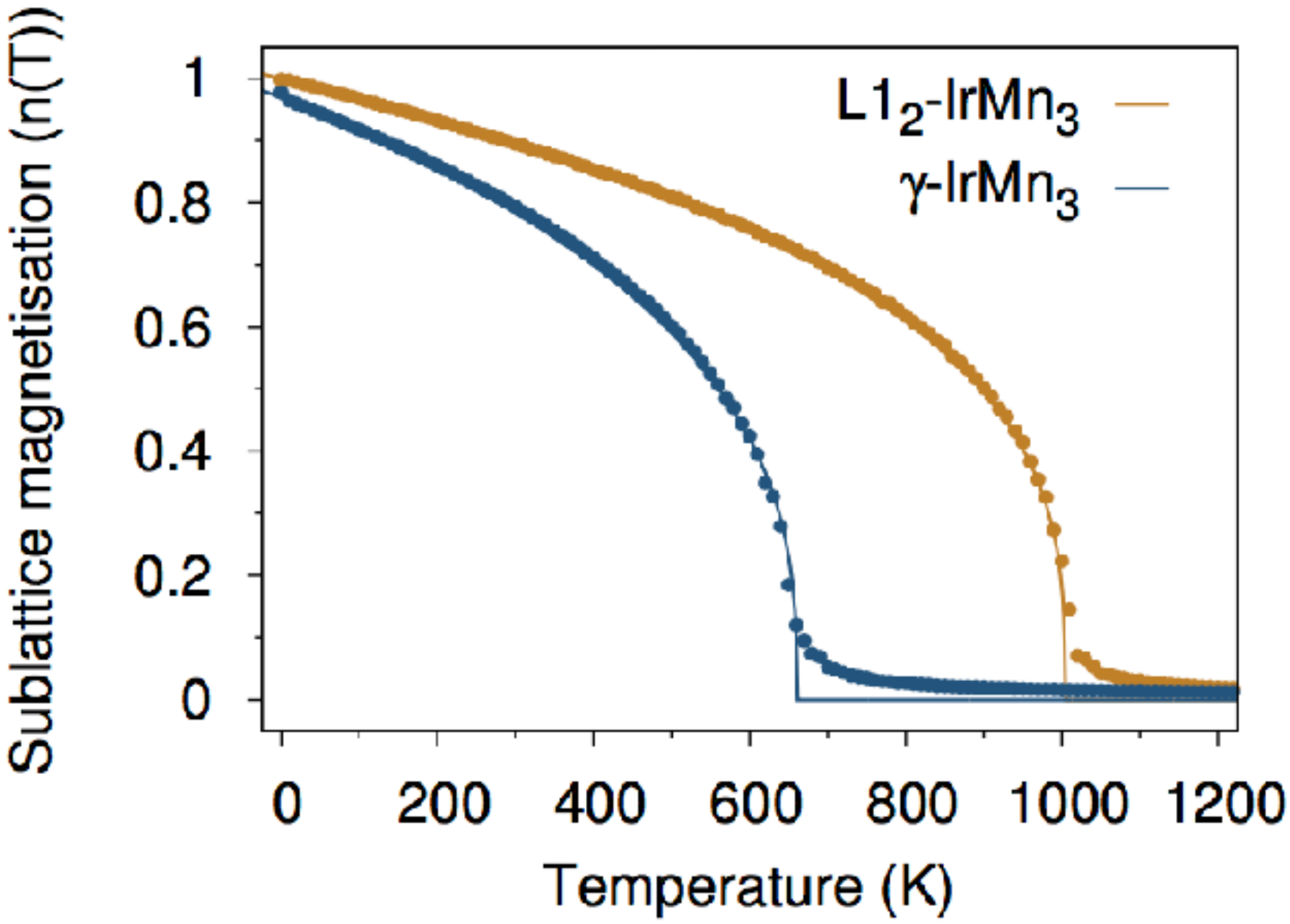


Disordered γIrMn$_3$

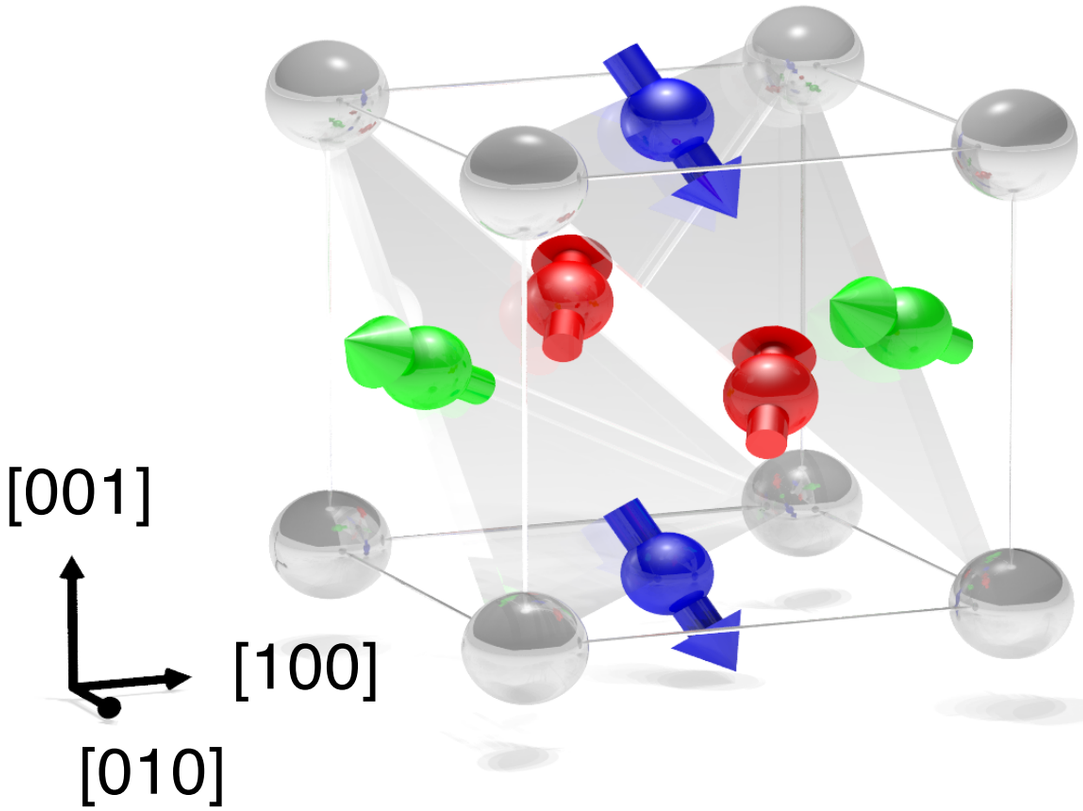


Ordered L1$_2$ IrMn$_3$

Field-cool simulations

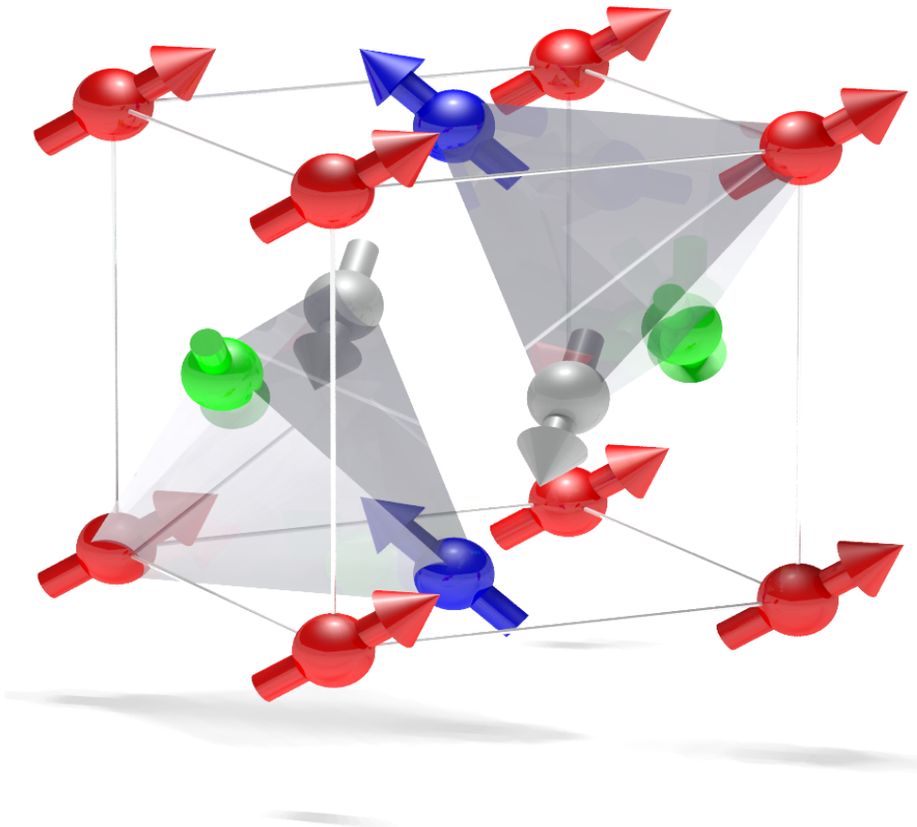


Magnetic Ground states



$L1_2$ - $IrMn_3$

Triangular (T1)



γ - $IrMn_3$

Tetrahedral (3Q)