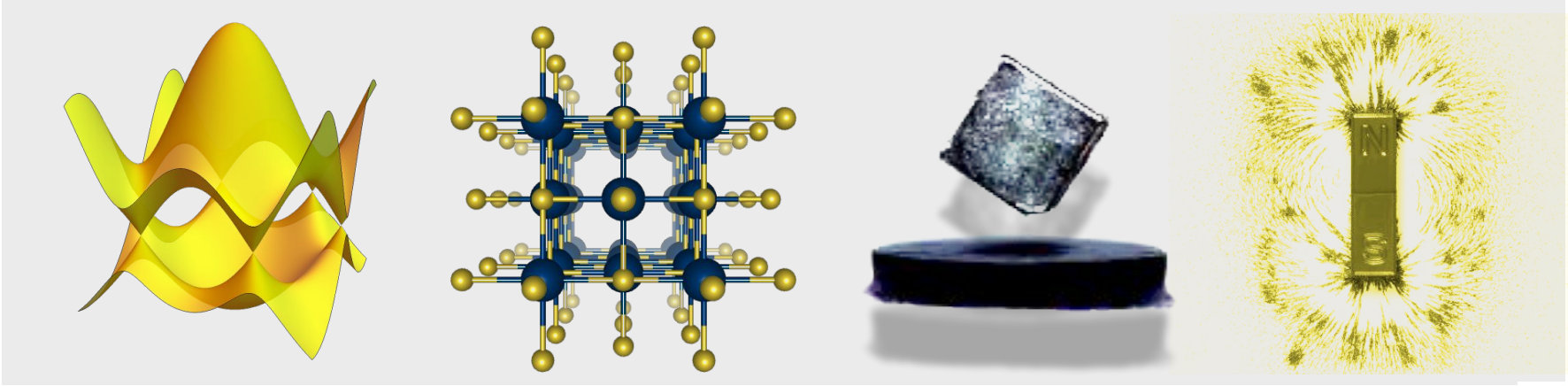
ESCOLA SÉRGIO MASCARENHAS DE FÍSICA DA MATÉRIA CONDENSADA

Hands-On 4 - Computational

Magnetic properties



SBF

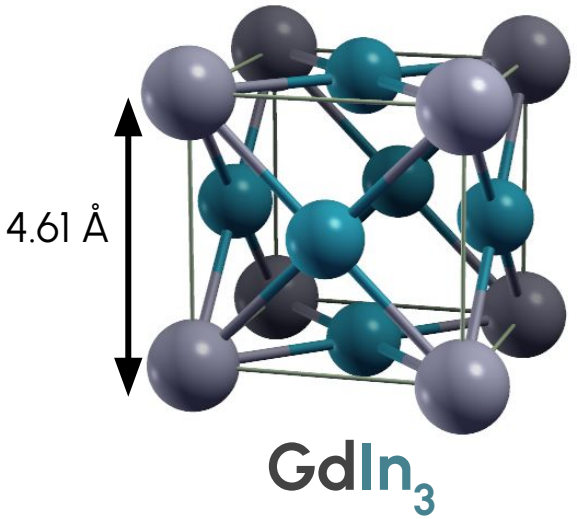
UFPE

Plan for today

- Basics of GdIn3
- Spin-polarized DFT
- Stable magnetic moments
- Ground state magnetic texture

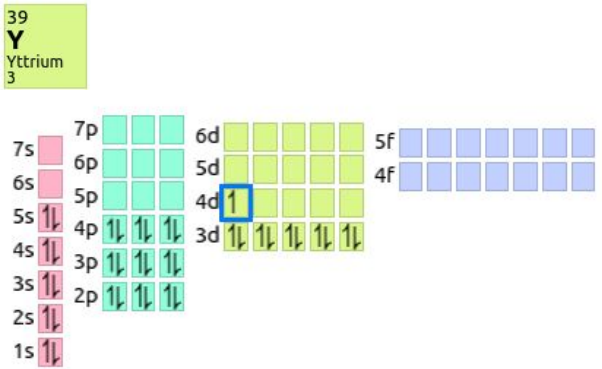
Basics of $GdIn_3$

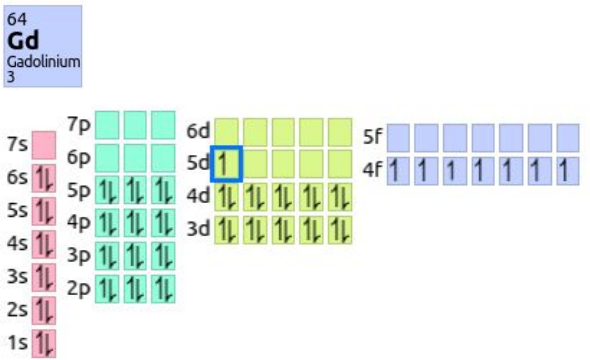
As YIn_3 is a non-magnetic material we will now study one of its close cousins: $GdIn_3$. The crystal structure is essentially the same, with the Yttrium atoms substituted by the Gadolinium ones.



The lattice parameter in YIn_3 is 4.58 Å while in $GdIn_3$ is 4.61 Å.

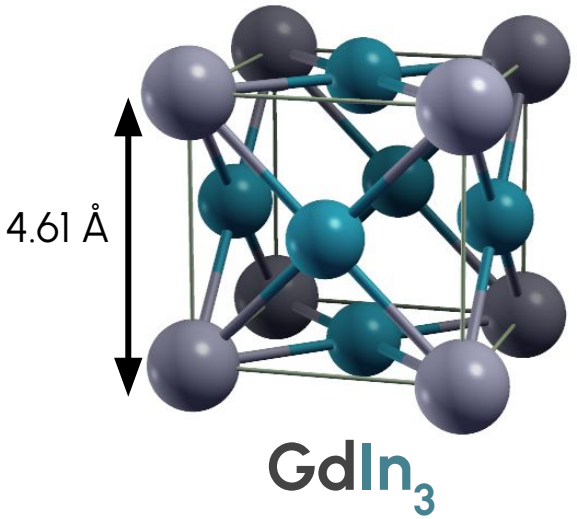
Both Yttrium and Gadolinium like to ionize into Y^{3+} and Gd^{3+}. Thus, unlike in the case of Y, we expect Gd to have <u>stable magnetic</u> moments arising from the partially filled 4f orbitals.





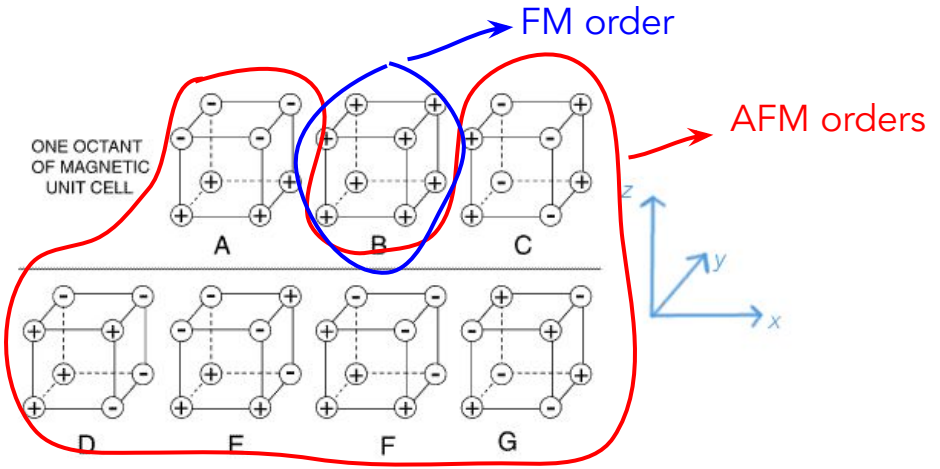
Basics of $GdIn_3$

As YIn_3 is a non-magnetic material we will now study one of its close cousins: $GdIn_3$. The crystal structure is essentially the same, with the Yttrium atoms substituted by the Gadolinium ones.



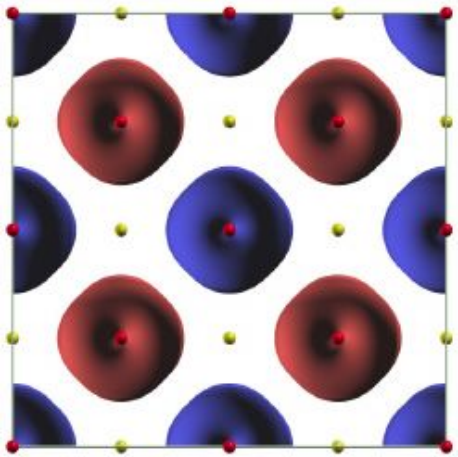
GdIn3 is experimentally known to be a magnetic conductor.

At high temperatures it is a paramagnet. Below ~45 K it acquires a long-range antiferromagnetic order (which AFM?).

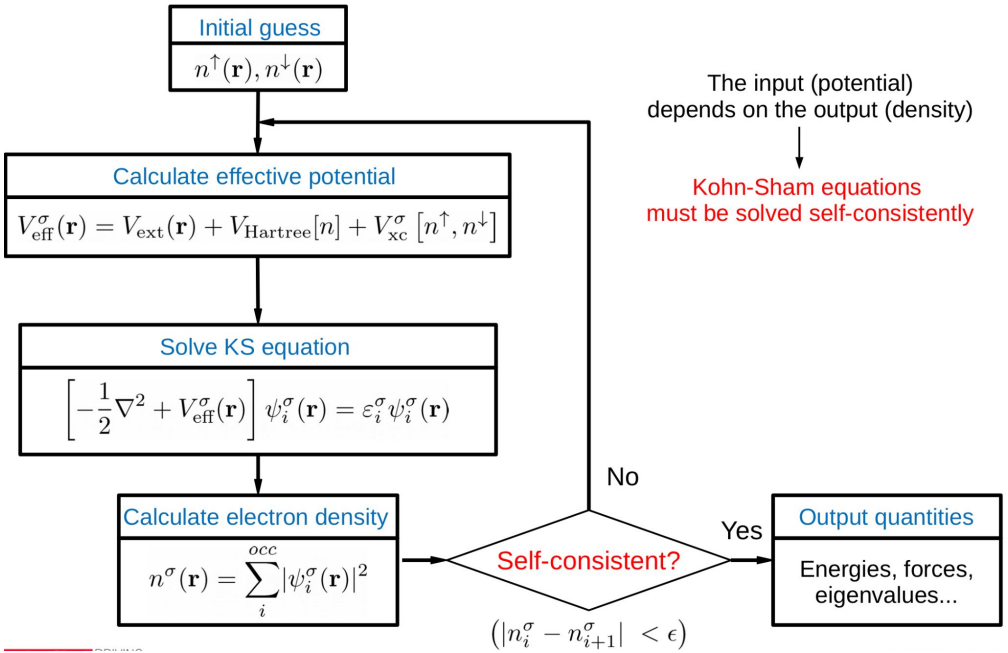


Spin-polarized DFT

Now we have two charge densities: one density for spin-up electrons and another for spin-down electrons. That translates into two self-consistent cycles coupled to each other.



Spin-density, $s=n_{\uparrow}-n_{\downarrow}$, in FeSe (red/blue is positive/negative s)



➔ Connecting to the VPN (Virtual Private Network)

```
>> sudo vpnc-connect /etc/vpnc/sdumont.conf --enable-weak-encryption
>> Enter password for login@146.134.0.14:
>> VPNC started in background (pid: ###)...
```

➔ Log in to SDummont:

```
>> ssh your_username@login.sdumont.lncc.br
>> password:
```

➔ Go to your scratch area:

```
>> cd /scratch/efmc24/your_username
```

➔ Copy files to you user area:

```
>> cp -r /scratch/efmc24/HandsOn_Material/day4 .
>> cd day4
>> ls
```

Checking if stable magnetic moments exist

Checking if stable magnetic moments exist

➔ First do an unpolarized spin calculation on a single unit cell system

```
>> cd 1_stable_MagMoms/1_unpol/
>> cat GdIn3.in
```

After looking into the GdIn3.in scf file submit the job

```
>> sbatch sub_GdIn3.srm
```

Once the calculation ends check the converged total energy

```
>> grep ! GdIn3*out
```

Checking if stable magnetic moments exist

➔ Second, do a spin polarized calculation on a single unit cell system (i.e. FM)

```
>> cd ../2_xyFM-zFM_sp1/
>> cat GdIn3.in
```

The "nspin=2" defines the spin-polarized calculation. The "starting_magnetization" indicates that atom 1 (the Gd) should start with a positive magnetization [important to break the symmetry] 0.056. This is written as a fraction of valence electrons. Gd has 18 valence electrons, so 1/18=0.05555556 means we have one more spin up than down. The "tot_magnetization=1" imposes that at each iteration the total magnetization is 1.

```
&SYSTEM
    …
    nspin=2,
    starting_magnetization(1) = +0.05555556,
    tot_magnetization=1,
    /
```

Checking if stable magnetic moments exist

Submit the job

```
>> sbatch sub_GdIn3.srm
```

Once the calculation ends check the converged total energy and magnetic moments

```
>> grep -e ! -e magn GdIn3*out
```

```
     atom:    1    charge:    16.1937 magn:    1.1600   constr:  0.0000
     atom:    2    charge:    11.8734 magn:     -0.0304 constr:  0.0000
     atom:    3    charge:    11.8734 magn:     -0.0304 constr:  0.0000
     atom:    4    charge:    11.8734 magn:     -0.0304 constr:  0.0000
!    total energy              =   -1916.03108877 Ry
```

This ferromagnetically ordered system is more/less stable than the non-magnetic one?

Checking if stable magnetic moments exist

➔ You can now check what is the most stable magnetic moment. Do the same calculation now for 'total_magnetization' values of 1, 3, 5, 7 and 9.

Start by copying "2_xyFM-zFM_sp1/" into the folder "3_xyFM-zFM_sp3/" and modify the magnetization definitions

```
>> cp -r 2_xyFM-zFM_sp1/ 3_xyFM-zFM_sp3/
>> cd 3_xyFM-zFM_sp3/ ; rm *out
>> nano GdIn3.in
```

```
&SYSTEM
    …
    nspin=2,
    starting_magnetization(1) = +0.16666667,
    tot_magnetization=3,
    /
```

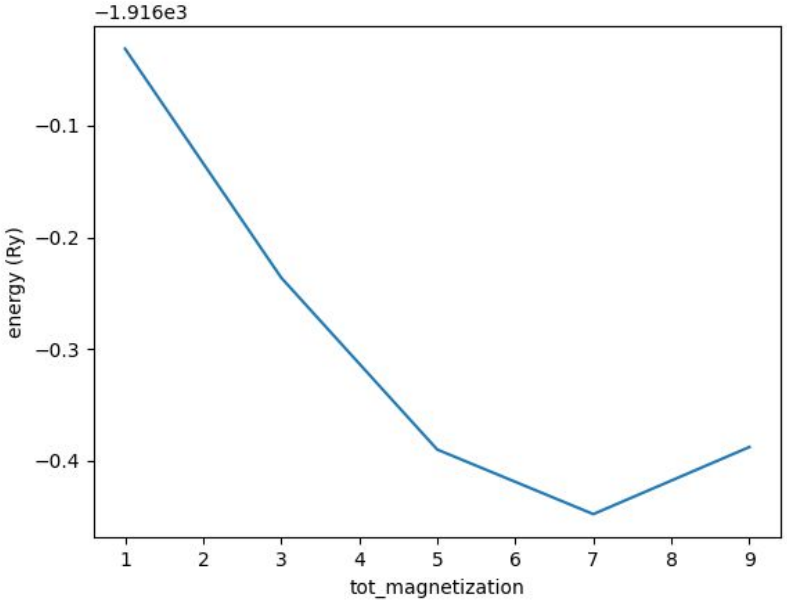
Checking if stable magnetic moments exist

Submit the job.

```
>> sbatch sub_GdIn3.srm
```

Do the same now for total_magnetization = 5, 7 and 9.

Once they are finished, collect total energies using grep, put the energies and the spin in a file 'data.csv' and then use the script 'plot.py' to generate a figure with the total energies of the different ferromagnetic states.



Ground state magnetic order

Ground state magnetic order

We have concluded that there are stable localized magnetic moments in the material. Now we want to find what is the lowest-energy magnetic texture.

Using a 2x1x1 supercell, we will now do SCF calculations for the unpolarized system, for the ferromagnetic, and for the antiferromagnetic order (xy-collinear-z-fm). Check the input.

```
>> cd ../2_magn_ground_state/3_xyCOL-zFM/
>> nano GdIn3.in
```

```
&SYSTEM
    …
    nspin=2,
    starting_magnetization(1) = +0.38888889,
    starting_magnetization(2) = -0.38888889,
    tot_magnetization=0,
    …
    /
```

Ground state magnetic order

```
ATOMIC_SPECIES
Gd1  1.00   Gd.paw.z_18.atompaw.wentzcovitch.v1.2.upf
Gd2  1.00   Gd.paw.z_18.atompaw.wentzcovitch.v1.2.upf
In   1.00   In.pbe-dn-kjpaw_psl.1.0.0.UPF

CELL_PARAMETERS angstrom
9.345                   0.0                     0.0
0.0                     4.6725                  0.0
0.0                     0.0                     4.6725

ATOMIC_POSITIONS angstrom
Gd1   0.0                     0.0                     0.0
In    2.33625                 2.33625                 0.0
In    2.33625                 0.0                     2.33625
In    0.0                     2.33625                 2.33625
Gd2   4.6725                  0.0                     0.0
In    7.00875                 2.33625                 0.0
In    7.00875                 0.0                     2.33625
In    4.6725                  2.33625                 2.33625

K_POINTS automatic
 3 6 6  0 0 0
```

Ground state magnetic order

What is the magnetic texture with the lowest total energy?

Can we give an estimate for the T_N? Yes! Assuming an Heisenberg model (which is wild approximation since this system should be governed by RKKY interactions)

$$\hat{H} = -J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

we know that the mean-field solution has a T_N that depends on the exchange coupling J,

$$T_N = \frac{zJS^2}{3k_B}$$

We equate the energy difference between the FM and AFM in the Heisenberg model to the difference in energy of those states in the ab initio calculation. From that we extract J.

$$J = \frac{\Delta E_{abinit}}{4S^2}$$

What is your estimate for T_N?