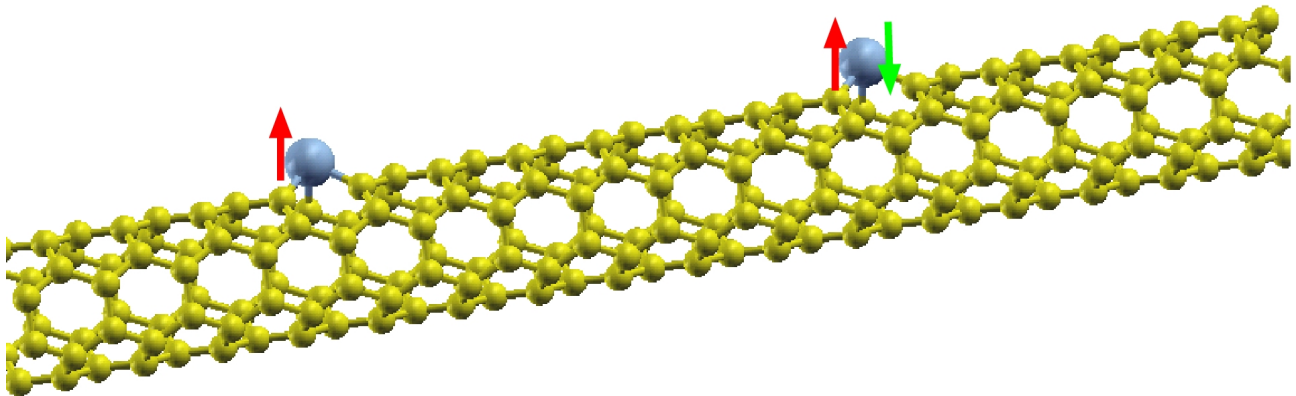


# DFT-NEGF based quantum transport simulations

## Day 2: CNT substitutionally doped with magnetic ions



The aim of this second DFT-NEGF tutorial is to use the code for a system of interest. We will investigate how substitutionally added magnetic impurities affect the transport properties. In particular, we will add 2 such impurities in the scattering region at different positions, and observe the 0 bias change in transmission for parallel and for antiparallel alignment of the impurities.

First the results for the pristine CNT will be presented. Then you will take those files as starting point and make separate directories where you will add the additional magnetic atoms.

In the Appendix B of this tutorial there is a short usage guide how to login, copy files and run on stampede. In the documentation for the Day1 there is the longer version.

### ***Logging in and copying files***

Login to stampede and xsede (see Day\_1 instructions if you forgot how to do it). In your home directory then execute

```
cp -r /work/02598/amaury/CNT .  
cd CNT
```

In this directory there are two subdirectories, one for the leads (CNT\_leads) and one for the pristine CNT scattering region (CNT\_pristine).

### **Magnetic systems**

So far all calculations were for non-magnetic systems. In this second part we will investigate the spin-polarization of current and transmission, and the change of resistance when spins of two magnetic centers are parallel and anti-parallel.

## Leads

Then change into the CNT\_leads directory, and submit the “submit.sh” job that will run the leads. Have a look at the “submit.sh” file: the main difference to the test runs for the first part is that now we run on 32 processors for the leads calculation. This is due to the fact that the system size is significantly larger than what considered yesterday.

```
cd ~/CNT/CNT_leads
sbatch submit.sh
```

The flag in the input file to switch on spin polarization in the calculation is the option SpinPolarized T.

## Scattering region

Each group will perform a calculation for a different magnetic atom configuration. Overall we will use 4 different magnetic ions (Mn, Co, Fe, Ni). Calculations will be performed for the single ions, and then for the 2 magnetic centres at 2 different distances. For these configurations with 2 magnetic centers the calculation will be run for parallel and antiparallel alignment of the magnetic moments.

In the “CNT” directory make a subdirectory where you will set up your scattering region for the specific assigned configuration. For example we will take the configuration with two Mn atoms in parallel configuration, so we will call the directory Mn\_Mn\_parallel.

```
mkdir Mn_Mn_parallel
```

Change into the directory for the pristine system, and copy the input.fdf file to the new directory, and change into the new directory

```
cd CNT_pristine
cp input.fdf ../Mn_Mn_parallel
```

In this directory there are also all the needed pseudopotentials (files with the .psf ending). Copy the pseudopotential for your magnetic atom in the new directory, in this case Mn.psf

```
cp Mn.psf ../Mn_Mn_parallel
```

Then change into the new directory

```
cd ../Mn_Mn_parallel
```

Here now edit the input.fdf file to add the magnetic atom.

In general, when self-consistency is achieved, the same files are output as for a non-spinpolarized calculation, however these files now contain additional data for the spin-

polarization. In particular, the file with the .TRC ending, which contains the data for the transmission coefficient,  $T$ , is now output in units of  $e^2/h$  (compared to  $2e^2/h$  for calculations without spin-polarization), since each spin-channel gives a maximum transmission of that value. The first column is the energy in eV, the second column the total transmission, the third column  $T$  for spin up, the fourth column  $T$  for spin down. The fifth (sixth) column contains the number of open channels in the electrodes for spin up (down). And finally the seventh and eight columns contain the up and down DOS for the scattering region (in this case we don't calculate the leads DOS, so it is not output). The file with the .RHO ending, which contains the charge density on a real space mesh, now contains data for both up and down spins, and so does the file with the .EMPDOS ending that contains the PDOS. Since the Hartree potential has no spin-dependence, the file with the .VH ending is unchanged compared to a non-spin-polarized calculation. If the get\_PDOS.sh script is run for a spin-polarized calculation, in each of the output files (one for each entry in the Input\_fm file) there are three columns, in the first there is the energy, and in the second one the PDOS for up-spins, and in the third one the PDOS for down-spins. The one for down-spins is multiplied with -1, so that it has a negative sign (this is the usual convention for plotting spin-polarized DOSs).

You will now have to replace a set of C atoms at defined positions with magnetic atoms. In the input file you have to change the NumberOfSpecies to 2, which tells the code that now there are 2 atomic species in the system (instead of 1). Then you have to add a line in the block ChemicalSpeciesLabel block, for Mn it is "2 25 Mn". This tells the code that the second species has atomic number 25 and is Mn. In general, all the atomic species used in the calculations are defined in this block.

In order to have consistent and comparable numbers for different groups, you will replace the atoms at the following positions:

1) the first atom at position

9.0716446604 11.469225786 12.3850000000

If you only put the single atom substitute this C atom. This atom has index 64.

2) The second atom at two possible positions:

a) 9.0716446604 11.0469225786 29.7240000000

This atom has index 148.

b) 9.0716446604 11.046617992 17.3390000000

This atom has index 88.

In this way they will have two different separations from the first atom.

For the magnetic atom atom, inside the block AtomicCoordinatesAndAtomicSpecies you have to replace the species index from C (species index 1) to the the one of the magnetic atom (species index 2). Each line of this block contains the x-coordinate in Angstrom of an atom (first entry), the y-coordinate (second entry) and the z-coordinate (third entry). The fourth number is an integer and is the atomic species index. Note that the text after the fourth column is not read by the code in this block, so arbitrary comments can be added.

For a relaxed configuration the magnetic atom shifts out of the CNT surface by about 0.9 Ang. You will not relax the atomic structure, but simply shift the y-coordinate of the top-most C atom by 0.9 Ang. In this calculation all atoms that will be substituted are in the top-most CNT C layer. Perform this substitution for as many C atoms that you need to replace (1 or 2) .

Finally, because this is a magnetic system, we need to set the initial spin of selected atoms. Assuming that the two Mn atoms have atom index 50 and 100 in the AtomicCoordinatesAndAtomicSpecies block (it will be different for every calculation), to this aim insert a block DM.InitSpin by adding the following lines at the end of the input.fdf file:

```
%block DM.InitSpin
```

```
50 +
```

```
100 +
```

```
%block DM.InitSpin
```

This tells the code that atoms with indices 50 and 100 (in this case the Mn atom) will be initialized with maximum spin along the up direction. This therefore corresponds to the parallel alignment. To initialize the atom in the down direction one needs to replace the “+” with a “-” (so in this case to set the AP configuration one needs to change the initialization of the atom 100 to “-”). Usually at self-consistency the magnitude of the spin will change from the initial value, but its direction will remain the same.

This concludes the setup. You can run the calculation in this directory by executing

```
sbatch submit.sh
```

If you edit the submit.sh script you will see that we ask for 64 processors, and also 5 hours of runtime. In general the calculation should take anything between half an hour and 1 hour.

While the calculation is running, execute “fdf2xyz\_xsf.sh input.fdf” to obtain the xyz and xsf files, transfer the file to your laptop, and then visualize the atomic structure, to check its correctness.

In general spin-polarized systems take more iterations to converge than non-spinpolarized systems. At selfconsistency, to check whether the system has indeed a net magnetic moment you can check the output file for a line with “Total Spin”, which contains the total magnetic moment of the simulation cell. From the command line you can also execute `grep "Total Spin" out` to extract this line.

Since the system is expected to be magnetic, plot the second column ( $T_{\text{total}}$ ), but also the third ( $T_{\text{up}}$ ), and the fourth ( $T_{\text{down}}$ ) as function of energy (the first column). If you use xmgrace to plot this you can execute

```
xmgrace -block 0.Fe_pc_P.TRC -bxy 1:2 -bxy 1:3 -bxy 1:4&
```

The transmission can be significantly different for up and down spins, depending on the system. Note the differences for your particular system

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Usually the transmission for two magnetic centers can be inferred to, at least qualitatively, from the one of the single impurities.

Plot also the PDOS for the two Fe atoms. First set up an appropriate Input\_fm file, and then execute get\_PDOS.sh

In this calculation you will also analyze the projected density of states (PDOS) on the magnetic atoms, which will help in understanding the shape of the energy dependent transmission. In order to get the PDOS printed you need to set the option "TRC.EMPDOS" to T. Calculate the PDOS for the shifted magnetic atoms using the get\_PDOS.sh script (see Appendix A for how to use the script). To run the script an input file is required, which tells the script for which atoms and orbitals to calculate the PDOS. A sample input file for this script, can be found in the directory for the pristine system, and is called "Input\_fm". It prints the PDOS for atoms 64, 88, and 148. Copy this file to the directory where you are running, and execute

```
~/bin/get_PDOS.sh 0.cntM.TRC.EMPDOS Input_fm 0
```

This generates 3 new files, one for each entry in the Input\_fm file, with the ending of the file corresponding to the string chosen in the Input\_fm script for each entry. For example, in this case the file "0.cntM.TRC.EMPDOS.atom\_64" is the PDOS of the 64rd atom in the system. In each of these files the first column is the energy in eV (the 0 is set to EF), and the second (third) column is the up (down) PDOS for that atom in units of states/eV.

For a single magnetic atom a quantity of interest is the spin-polarization around the Fermi energy, which determines the low bias spin polarization of the current. We define it as

$$P(E_F) = (T_{\text{up}} - T_{\text{down}}) / (T_{\text{up}} + T_{\text{down}})$$

Evaluate this number for your system if you have only one magnetic center in the cell:

$$P(E_F) = \underline{\hspace{2cm}}$$

In the case with two magnetic centers the relative orientation of the spins on the two atoms will critically affect the transmission. For collinear spin alignments there are two options: either the spins of the two atoms are parallel to each other (P configuration), or anti-parallel (AP configuration). The normalized difference in the current for the two configurations

$$MR = (I_P - I_{AP}) / (I_P + I_{AP}),$$

is usually referred to as magnetoresistance (MR). Here  $I_P$  is the current for the P configuration, and  $I_{AP}$  is the current for the AP configuration. With this definition the MR is bound between -1 and 1. A commonly used alternative definition is where one divides the difference in currents only by the smaller of the two. With this alternative definition the MR can go from minus infinity to plus infinity. A large MR is a key factor in many devices such as magnetic hard disc drives read heads.

For small bias voltage the current is simply  $I = T(E_F) \cdot V$ , so that we get a low bias approximation for the MR by

$$MR(\text{small bias}) = [T(E_F; P) - T(E_F; AP)] / [T(E_F; P) + T(E_F; AP)]$$

We will calculate this quantity in this tutorial.

Then evaluate the small bias MR with above equation

MR(small bias)=\_\_\_\_\_

This value will depend on the relative positions of the two magnetic centers.

If the MR would be evaluated at energies different from  $E_F$ , can you find energies from the transmission graph where the MR is very large, if so at what energies?

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Once you have evaluated all the data, you will need to copy the main files to a shared directory (or send an email to [runggeri@tcd.ie](mailto:runggeri@tcd.ie)). The files are "input.fdf", the TRC file, the xyz file with the atomic structure, and the PDOS file for the magnetic atoms.

## Appendix A: Using the get\_PDOS.sh script

The shell script get\_PDOS.sh prints out a usage guide if called without arguments. It needs two input files:

1)file.PDOS or file.TRC.EMPDOS (the name is arbitrary): this file contains the output from a siesta or smeagol calculation for the PDOS.

2)Input\_fm: input file for get\_PDOS.sh, that tells the script for which orbitals it should print the PDOS. There should not be any empty lines in the file, and for each atom where the PDOS should be printed add 3 lines:

a)the first starts with a "#" character, and then followed by some arbitrary text. The text is then used as part of the output file name, and also in the xmgrace figure, for that particular orbital.

b)the index of the atom in the siesta input file

c)The number "0".

Note: in principle the input file can have more options, to print orbital dependent PDOSs, but this is not needed for the tutorial.

Here are the contents of an example input file Input\_fm (this can be used for example 1, exercise 1):

```
#Au_chain1
```

```
1
```

```
0
```

```
#Au_chain2
```

```
2
```

```
0
```

```
#Au_chain3
```

```
3
```

```
0
```

```
#Au_chain4
```

4

0

#Au\_chain5

5

0

## Appendix B: quick stampede usage guide

In order to be able to login on stampede you had to apply for an account and password as per instructions sent via email by Mark Pederson. In the following we assume that you have your account and password set up.

The procedures for connecting to the machine are different for linux and windows computers/laptops.

To login to stampede follow a 2 step process. Note however that some users might have the account setup for direct login. First login to the host “login.xsede.org” (xsede in short) with your user name.

### Linux

In linux open a terminal and type

```
ssh -Y username@login.xsede.org
```

where username is your user name. Once you enter your correct password you are logged in.

### Windows

On a windows machine run “putty.exe” or the ssh client of your choice, and enter the hostname in the appropriate field, and then it will ask you for username and password. Once these are entered correctly you will be logged in.

The xsede host is just an intermediate computer, from which you then login to the cluster stampede, where you will run the calculations. To login to stampede from xsede type

```
gsissh -p 2222 stampede.tacc.xsede.org
```

which will log you in to stampede without asking for a further password.

To submit a job script on stampede execute

```
sbatch submit.sh
```

This will then submit the job to the queue. To check the status of the job you can run

```
squeue -u username
```

### *Copying files to your laptop*

To copy files from the stampede cluster to your laptop computer you have to use a 2 step scp or

sftp. To scp the files from stampede to your laptop is also a 2 step process. First login a second time to xsede from your laptop (see above how to do this). Then on your laptop open e.g. a graphical user interface for sftp/scp, and open a connection to xsede. For linux the “filezilla”, program is suggested, and for windows winscp (or filezilla). You will first transfer the files from stampede to xsede, and then from xsede to your desktop.

To transfer files from stampede to xsede, connect to xsede with ssh, and then from within that terminal write (assuming you want to copy the input.fdf file from the home directory of stampede into the current directory):

```
gsiscp -P 2222 stampede.tacc.xsede.org:input.fdf
```

This will put the input.fdf file on xsede, and you can then transfer it with winscp/filezilla to your laptop.