

Dr. Jan Wilhelm

<https://www.uni-regensburg.de/physik/evers/teaching/comp-nano-bose-2021/index.html>

## Computational Nanoscience: Exercise Sheet No. 9

Please note that the longest calculation in (c) takes around an hour. All other calculations are quick (few minutes). For a full understanding of the `aitranss` (ab-initio transport simulations) code that you will use on this sheet, the lecture material from 15.6 and 15.7 may be helpful. All questions however can be also answered with the knowledge from 15.1 to 15.5.

### Exercise 9.1: Getting started with `aitranss`

- (a) Copy the structure of a junction and scripts to convert geometries to your directory:

```
scp phy318:/loctmp/comp_nanoscience/05_sheet_9/1_KS-DFT/geometry.in .
scp phy318:/loctmp/comp_nanoscience/aims2xyz.x .
scp phy318:/loctmp/comp_nanoscience/xyz2aims.x .
```

Convert the structure to the xyz format by

```
./aims2xyz.x geometry.in > geometry.xyz
```

and report the structure in your solution.

- (b) Copy also the FHI-aims control file to your directory,

```
scp phy318:/loctmp/comp_nanoscience/05_sheet_9/1_KS-DFT/control.in .
```

The keyword `output_aitranss` is important since it enables the printing of specific files that are needed by the `aitranss` code to compute the total transmission coefficient  $\mathcal{T}(E)$ .

Which basis set do we use? What kind of calculation are we doing with this input?

- (c) Execute the calculation with

```
nohup mpirun -np 4 ~/aims.x > aims.out &
```

This calculation takes around an hour. The `nohup` command lets the calculation run in the background. The output is written to the file `aims.out`. You can check whether the calculation is still running by entering `top` that reports all the running processes on the computer you are working on. Also you can check the status of the calculation by viewing the output file `aims.out`. After the SCF is converged, report the HOMO-LUMO gap. Why is the HOMO-LUMO gap that small?

- (d) Now, we use the FHI-aims output to perform a transport calculation (as described in Sec. 15.7 of the lecture). For doing so, we have to define a plane in each electrode where we add the self-energy. The plane is defined by providing three gold atom numbers that span such a plane. You can display the gold atom numbers in avogadro by clicking on `Display settings` and activating `label`. For our case, the we can choose the atom number 34, 36 and 40 for one plane and 29, 37, 38 for the other plane. Provide in your solution alternative atomic numbers defining these planes.
- (e) Please copy two executables that belong to `aitranss` to you home directory:

```
scp phy318:/loctmp/comp_nanoscience/05_sheet_9/2_aitranss/tcontrol.aims.x ~
scp phy318:/loctmp/comp_nanoscience/05_sheet_9/2_aitranss/aitranss.060914.x ~
```

Before executing `aitranss`, we create the `aitranss` input file `tcontrol` by entering

```
~/tcontrol.aims.x -lsurc 34 -lsurx 36 -lsury 40 -rsurc 29 -rsurx 37 -rsury 38
-nlayers 2 -ener -0.4 -estep 0.001 -eend 0.0
```

Ater executing the command, the file `tcontrol` is written. The first six numbers define the outermost planes of the junction, see FHI-aims manual, section 5.3.3 *How to create a mandatory file tcontrol*. `-nlayers 2` determines that we use a two atomic layers in each electrode to apply the self-energy (see Sec. 15.7 for theoretical background). `-ener  $E_1$  -estep  $dE$  eend  $E_2$`  (unit: Hartree (H),  $1 \text{ H} = 27.211 \text{ eV}$ ) defines the energy window  $[E_1, E_2]$  and energy step  $dE$  to calculate the total transmission function  $\mathcal{T}(E), E \in [E_1, E_2]$ .

For computing  $\mathcal{T}(E)$  from an `aitranss` calculation, enter

```
~/aitranss.060914.x
```

inside the directory where the output of your calculation from (c) is located. A file `TE.dat` should be written with the first four lines being

```
#non-spin-polarized calculation
#bias = 0.000000 V efermi = -0.172517412465 H
# E [Hartree] E-EF [eV] T(E) per spin
-0.4000000000 -6.19011604 0.9794610327E+00
```

Report the fifth line to your solution pdf and provide a plot of  $\mathcal{T}(E)$ .

- (f) The `TE.dat` file reports the Fermi level of the junction. Have a look at the HOMO and LUMO level from the FHI-aims output `aims.out` and provide the formula that was used for computing the Fermi level in the file `TE.dat`.
- (g) What is the conductance of the junction when applying an infinitesimally small bias voltage?
- (h) Based on `TE.out`, numerically compute the current  $I$  that is flowing through the junction when applying a bias voltage of 0.5 V between both electrodes. Assume a temperature of zero Kelvin and that the Fermi levels of both electrodes are shifted symmetrically, i.e. by +0.25 eV and -0.25 eV.
- (i) Which current is flowing, if we keep the chemical potential of the left electrode fixed while we lower the chemical potential of the right electrode by 0.5 eV? Which current is flowing, if we keep the chemical potential of the right electrode fixed while we lower the chemical potential of the left electrode by 0.5 eV?