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Summer term 2021
Discussion on: 10 June 2021

http://www.physik.uni-regensburg.de/forschung/evers/courses/2021/comp_nanoscience.phtml

Computational Nanoscience: Exercise Sheet No. 7

Exercise 7.1: FHI-aims setup and geometry optimization

From now on, we will use the FHI-aims software package for our computations. More information on FHI-aims can be found on

https://aimsclub.fhi-berlin.mpg.de/

For running FHI-aims, create a new directory in your home directory (the home directory can be abbreviated with ~) and enter this directory:

```
mkdir ~/FHI_aims
cd ~/FHI_aims
```

Copy the executable, the aims manual and geometry conversion scripts to your directory:

```
scp phy318:/loctmp/comp_nanoscience/aims.x .
scp phy318:/loctmp/comp_nanoscience/FHI-aims.pdf .
scp phy318:/loctmp/comp_nanoscience/xyz2aims.x .
scp phy318:/loctmp/comp_nanoscience/aims2xyz.x .
```

It can be convenient, to create another directory somewhere else where you run the FHI-aims calculations, for example:

```
mkdir ~/calculations_FHI_aims
cd ~/calculations_FHI_aims
```

This exercise requires the theory of Chapter 12 on potential energy surfaces from DFT.

(a) In your calculation directory, create a new directory and copy the control file of FHI-aims into this directory by the command

```
scp phy318:/loctmp/comp_nanoscience/control.in .
scp phy318:/loctmp/comp_nanoscience/geometry.in .
```

Have a look at `geometry.in` and observe that we have a planar H_3O^+ ion. You can transform the structure from `geometry.in` to an xyz file via

```
~/FHI_aims/aims2xyz.x geometry.in > H3O+_initial.xyz
```

Convince yourself that all atoms are located in a plane (e.g. looking at the coordinates in the files or by copying the file to your computer and viewing it with avogadro).

Have a look at the the file `control.in`. Most important are the first 5 lines:

```
xc pw-lda
charge 1.0
spin none
sc_iter_limit 300
relax_geometry trm 1E-3
```

that correspond to using the LDA xc functional, a positive charge for H_3O^+, a closed-shell calculation, a maximum of 300 SCF iterations and a criterion for the geometry optimization.

The executable `aims.x` can perform DFT calculation for a single geometry ("single-point DFT calculation") and geometry optimizations. By specifying the `relax_geometry` keyword in `control.in`, we activate the geometry optimization. Perform a geometry optimization by entering

```
mpirun -n 1 ~/FHI_aims/aims.x | tee aims.out
```

The geometry after completing the geometry optimization is reported in `geometry.in.next_step`. Do the atoms still lie in one plane?

(b) Search for the forces in the FHI-aims output (`aims.out`). Focus on Hellmann-Feynman forces and Pulay forces. The three displayed rows correspond to the forces in x-, y- and z-direction. Which force type (Hellmann-Feynman or Pulay) is larger?

(c) Do forces get smaller in the geometry optimization? Report the forces after the first DFT calculation and the last force after the last DFT calculation.

(d) Why do the forces have very small z-component?

(e) Start a new geometry optimization with FHI-aims. Use the start geometry from (a), but change the z-component of the oxygen atom to 0.1. What is the difference of the relaxed geometry from (e) to the relaxed geometry from (a)?

(f) Is the geometry from (a) or (e) the global minimum? How can you judge based on numbers from the FHI-aims output?

(g) Explain, why the geometry optimizations from (a) and (e) yield different geometries and give some advice how starting geometries for a DFT geometry optimization should be chosen.

Exercise 7.2: Numerical convergence in FHI-aims

Have a look at the original publication on the DFT implementation in FHI-aims, V. Blum *et al.*, Comp. Phys. Commun. **180**, 2175-2196 (2009), and download it (e.g. via UR VPN).

(a) What is the form of the basis in FHI-aims?

(b) What is the main advantage and the main drawback of the FHI-aims basis compared to the Turbomole basis?

(c) Have a look at Fig. 3 in the FHI-aims implementation paper and at the `control.in` file you have used. Which basis set have you used in your geometry optimizations in (a) and (e)? How can you check basis set convergence in FHI-aims?