

# Exercises - Friday

March 22, 2006

Topics: NMR, van der Waals, Wannier orbitals & centres & ELF

## Start

- In the shell execute:

```
cd <your-work-directory>
mkdir H2O
cd H2O
cp ~/Job_sub.cmd .
cp ~/H2O-nmr.inp input
```

- Output comes in file 'output'

## 1 NMR shield tensor for H<sub>2</sub>O

1. Get CH4.inp and H2O.inp from the homedirectory
2. Optimise geometry of H<sub>2</sub>O
3. Optimise geometry of CH<sub>4</sub>
4. Carry out NMR calculations with the LINEAR RESPONSE keyword in the control section and the following section

```
&RESP
  NMR ISOLATED
  0.1
  CONVERGENCE
  0.0005
&END
```

5. compare your results to Literature values (GIY)
6. what happens to the shift if you change the hybridization state of the oxygen (tip: protonate the water molecule to get H<sub>3</sub>O<sup>+</sup>)? What happens to the shift if you change the bondlength?

## 2 vdW-correction scheme

Compute the energy of interaction curve for the ethylene dimer using BLYP, the empirical correction, and the atom centered correction.

- copy the file Ethyl.in from home
- optimize the geometry of the ethylene dimer constraining inter molecular distance (z) of the carbons, thus moving only the hydrogen atoms along all x,y,z axes (view structure with vmd to check it first)
- keep intramolecular structure fixed and vary only the intermolecular distance for values between 2.8 and 4.3 Å. Is your cell size big enough for that? For which cell size exhibits your dimer converged energies of interaction? Why is there no BSSE-error in CPMD?
- Now, include the following section into your calculations:

```
&VDW
  VDW CORRECTION
  1
  C6 1 2 -92.99225 4.4425 1
&END
```

- Next replace your carbon pseudopotentials by a file which contains the following:

