NCIPLOT4

1. Looking at non covalent interactions in small molecules

a) Run the following input to visualize the NCI file for benzene dimer:

```
1 !number of files to be rea
BenzeneDimer.wfn !name(s) of the files
```

b) Load the file `BenzeneDimer.vmd` on `vmd` to see the NCI results. What interaction do you see?

c) Different types of calculations are possible with NCIPLOT. We will estimate non covalent interactions with a promolecular density, so just the position of the atoms is needed. You can check the geometry input in `FormacDimer.xyz`. Follow the same procedure as in benzene dimer to visualize Formic acid dimer. Several interaction types appear. Which ones?

d) Use the `python` code `nci_rangeFP.py.` Type "python nci_rangeFP.py" and follow the calls interactively:

"FormacDimer"
"E"
-0.02
0.02.
What have you done? Can you explain the values "-0.02" and "0.02"? What happens if you write "I" instead of "E"?

e) NCIPLOT can be used to analyze strong interactions too. Analyze the interactions in LiF (lif.wfn). This interaction is stronger than common non-covalent interactions, so you will need to adjust the cutoffs. Use `GNUPLOT` (or other plotting code) to plot s(ρ). At which density appears the Li-F ionic interaction? Use this information with the keyword `CUTPLOT` to visualize the Li-F interaction:

```
CUTPLOT ?? 0.5
```

2. Analysing intermolecular interactions in bigger systems

a) Analyze the interactions between the active site of the 2v5x protein and its ligand. (files: `2v5x-within5.xyz` and `ligand.xyz`). What interactions are responsible for the stabilization?

b) In order to accelerate the calculation you can use the adaptative grid (4 subdivisions) and a good resolution for a nice rendering:

```
CG2FG 4 8 4 2 1
```

c) In these cases we are usually just interested in the intermolecular interactions. Use the adaptative grid from section 2b) and the following keyword to look exclusively at intermolecular interactions and compare the result with the one from a normal run:

```
intermolecular 0.9
```

d) In order to quantify the interactions you can carry out an integration of the charge within the NCI region. We will look at a dimer (monomers A and B) of the Aβ40 extracted from the fibril structure (abeta40dimerA_1micros_10.xyz and abeta40dimerB_1micros_10.xyz). We can for

example look at the three coloring ranges, attractive (-0.1< ρ <0.02), repulsive (0.02< ρ <0.1) and van der Waals (-0.02<ρ<0.02) with the following input:

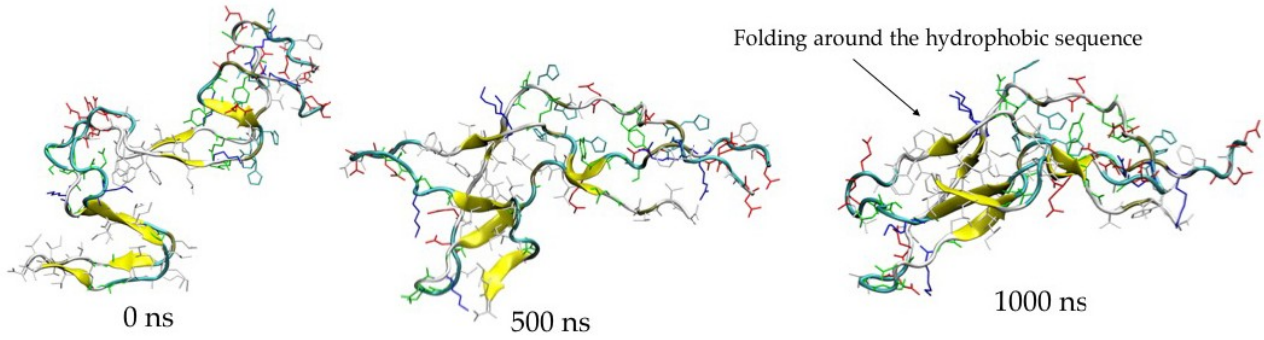
```
2
abeta40dimerA.xyz
abeta40dimerB.xyz
INTERMOLECULAR
CUTOFFS 0.2 1.0 ! following intervals for s=0.1 and ρ=0.2
CG2FG 4 8 4 2 1
INCREMENTS 0.2 0.2 0.2 !smaller number of points
OUTPUT 1 !dont print the cube files
RANGE 3
-0.1 -0.02
-0.02 0.02
0.02 0.1
```

Take the values for n=1, which correspond to the charge enclosed by the intermolecular interactions up to s=1.0 and fill in this table:

Interaction type	**Charge (n=1)**
Atractive	
vdW	
Repulsive	

3. Molecular dynamics

a) Now we are going to make use of the fat focus in a classical MD. The test system is a dimer (A and B) of the Aβ42 extracted from the fibril structure of PDB 2NAO (`abeta42dimerA_1micros_n.xyz` and `abeta42dimerB_1micros_n.xyz`). The initial geometry of the dimer is that of the fibril; a 1μs dynamics in explicit solvent (water) simulation is run to observe the folding (the yellow pieces in the figure represent the β-sheet secondary structure). What interactions do you expect from the intra and intermolecular point of view at the following steps?



b) We will look at steps every 10 snapshots. Evaluate the evolution of the integrals along the MD What do you observe? Does this coincide with your predictions?