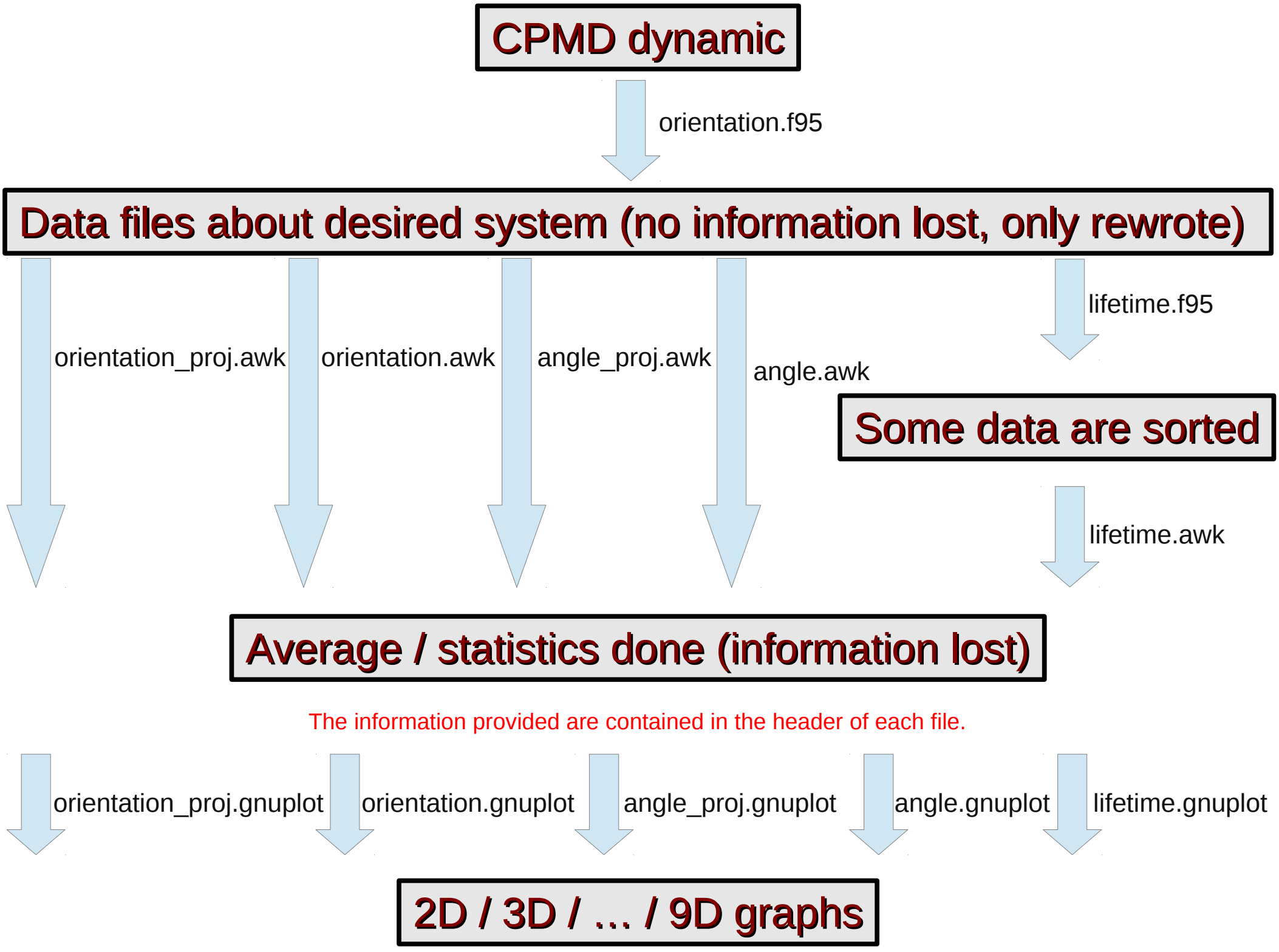

CPMD dynamic
orientation.f95
Data files about desired system (no information lost, only rewrote)
orientation_proj.awk
orientation.awk
angle_proj.awk
angle.awk
lifetime.f95
Some data are sorted
lifetime.awk
Average / statistics done (information lost)
The information provided are contained in the header of each file.
orientation_proj.gnuplot
orientation.gnuplot
angle_proj.gnuplot
angle.gnuplot
lifetime.gnuplot
2D / 3D / ... / 9D graphs

Practice

```
rekhatib@cpmd01:~/tmp$ orientation < input_orientation
 Name of the input file
 There are         444 atoms.

 Symbol of the central atom:
 How many ligands?
 Symbol of the ligand number           1 :
 Minimal distance defining this O-H:
 Maximal distance defining this O-H:
 Symbol of the ligand number           2 :
 Minimal distance defining this O-H:
 Maximal distance defining this O-H:
 Do you accept to have one ligand shared by two central atom? (y/n - default n)

 !!!    Only MXn molecules with the 'good' bonds will be taken into account    !!!
 !!!    MXn-1, MXn+1 or MXn with short bonds will not be taken into account    !!!
 !!!If a X is shared by 2 M, none of these molecules will be taken into account!!!

Label of the ligand H with rmin=  0.90Ang and rmax=  1.10Ang: H1 H2

 Write the root name of the output files
 The output files will be:
     -CaF2_H2O_neutral_xO.dat
     -CaF2_H2O_neutral_yO.dat
     -CaF2_H2O_neutral_zO.dat
     -CaF2_H2O_neutral_vxH1.dat
     -CaF2_H2O_neutral_vyH1.dat
     -CaF2_H2O_neutral_vzH1.dat
     -CaF2_H2O_neutral_vxH2.dat
     -CaF2_H2O_neutral_vyH2.dat
     -CaF2_H2O_neutral_vzH2.dat
     -CaF2_H2O_neutral_life-over.dat
     -CaF2_H2O_neutral_life-under.dat

 What are the crystal parameters? (Ang)

 O atoms:
 How do you want to select these atoms? (ALL/NUMBER)

 H atoms:
 How do you want to select these atoms? (ALL/NUMBER)

 Starting step (default:       14868 )
 Final step (default: end of file)
 Step       16000  treated.
   99.928835321906604      % of O have the good ligands.
```

This is how the molecules are selected. The 3rd line can not appear (depends on you)

Explanation about the ligand / file names

```
rekhatib@cpmd01:~/tmp$ emacs input_lifetime
rekhatib@cpmd01:~/tmp$ lifetime < input_lifetime
 Filename of the lifetime file
 Filename of the z-projection of the central atom
 Cell parameter along the normal axis (Ang)
 Center of the vacuum/solid slab (Ang)
 Filename of the output
 For the lifetime windows, do you want:
    -a constant timestep (1)
    -a constant ratio 'timestep' over 'average value' (2)
 The first lifetime division starts at 1.
 What is the beggining of the second lifetime windows (Real accepted. Default: 1.01):
 Step       15000 treated.
 Step       16000 treated.

 Data recorded. Sorting the data.
          50  over          387  lifetime windows treated.
         100  over          387  lifetime windows treated.
         150  over          387  lifetime windows treated.
         200  over          387  lifetime windows treated.
         250  over          387  lifetime windows treated.
         300  over          387  lifetime windows treated.
         350  over          387  lifetime windows treated.

 Data sorted. Spliting the data.
```

The sorting algorithm is an insertion algorithm (VERY slow when we have many values). If you select a huge timestep, maybe you will need several hours to treat your data. I will try to change the algorithm.

A kind of “bar chart” will be done. To calculate the width of each bar there are two possibilities:
-The width is constant (very intuitive way to split the data)
-The width is proportional to the average lifetime of the bar

In the first case, we will have, for example, 1) a bar to describes the lifetime between 10 and 20 steps and 2) another one to describe the lifetime between 1000 and 1010 steps.

In the second case, we will have for example, 1) a bar to describes the lifetime between 10 and 20 steps and 2) another one to describe the lifetime between 1000 and 2000 steps.

Awk commands without bash script

The scripts work only for MX2 molecules (like H2O for example)

```
awk -f ~/bin/__gnuplot/lifetime.awk CaF2_H2O_neutral_lifetime.dat > CaF2_H2O_neutral_life_boxplot.dat
```

```
awk -v a=34 -v b=11.59 -v c=13.38 -v div=0.1 -v x0=CaF2_H2O_neutral_xO.dat -v
y0=CaF2_H2O_neutral_yO.dat -v z0=CaF2_H2O_neutral_zO.dat -v x1=CaF2_H2O_neutral_vxH1.dat -v
y1=CaF2_H2O_neutral_vyH1.dat -v z1=CaF2_H2O_neutral_vzH1.dat -v x2=CaF2_H2O_neutral_vxH2.dat -v
y2=CaF2_H2O_neutral_vyH2.dat -f ~/bin/__gnuplot/orientation.awk CaF2_H2O_neutral_vzH2.dat >
orientation.dat
```

```
awk -v param=34 -v div=0.1 -v axis=CaF2_H2O_neutral_xO.dat -v x1=CaF2_H2O_neutral_vxH1.dat -v
y1=CaF2_H2O_neutral_vyH1.dat -v z1=CaF2_H2O_neutral_vzH1.dat -v x2=CaF2_H2O_neutral_vxH2.dat -v
y2=CaF2_H2O_neutral_vyH2.dat -f ~/bin/__gnuplot/orientation_proj.awk CaF2_H2O_neutral_vzH2.dat >
orientation_proj.dat
```

```
awk -v a=34 -v b=11.59 -v c=13.38 -v div=0.1 -v x0=CaF2_H2O_neutral_xO.dat -v
y0=CaF2_H2O_neutral_yO.dat -v z0=CaF2_H2O_neutral_zO.dat -v x1=CaF2_H2O_neutral_vxH1.dat -v
y1=CaF2_H2O_neutral_vyH1.dat -v z1=CaF2_H2O_neutral_vzH1.dat -v x2=CaF2_H2O_neutral_vxH2.dat -v
y2=CaF2_H2O_neutral_vyH2.dat -f ~/bin/__gnuplot/angle.awk CaF2_H2O_neutral_vzH2.dat > angle.dat
```

```
awk -v param=34 -v div=0.1 -v axis=CaF2_H2O_neutral_xO.dat -v x1=CaF2_H2O_neutral_vxH1.dat -v
y1=CaF2_H2O_neutral_vyH1.dat -v z1=CaF2_H2O_neutral_vzH1.dat -v x2=CaF2_H2O_neutral_vxH2.dat -v
y2=CaF2_H2O_neutral_vyH2.dat -f ~/bin/__gnuplot/angle_proj.awk CaF2_H2O_neutral_vzH2.dat >
angle_proj.dat
```

Awk commands with bash script (optional but so useful)

The scripts work only for MX2 molecules (like H2O for example)

awk -f ~/bin/__gnuplot/lifetime.awk CaF2_H2O_neutral_lifetime.dat > CaF2_H2O_neutral_life_boxplot.dat

~/bin/__gnuplot/orientation.sh 34 11.59 13.38 0.1 CaF2_H2O_neutral_xO.dat CaF2_H2O_neutral_yO.dat CaF2_H2O_neutral_zO.dat CaF2_H2O_neutral_vxH1.dat CaF2_H2O_neutral_vyH1.dat CaF2_H2O_neutral_vzH1.dat CaF2_H2O_neutral_vxH2.dat CaF2_H2O_neutral_vyH2.dat CaF2_H2O_neutral_vzH2.dat > orientation.dat

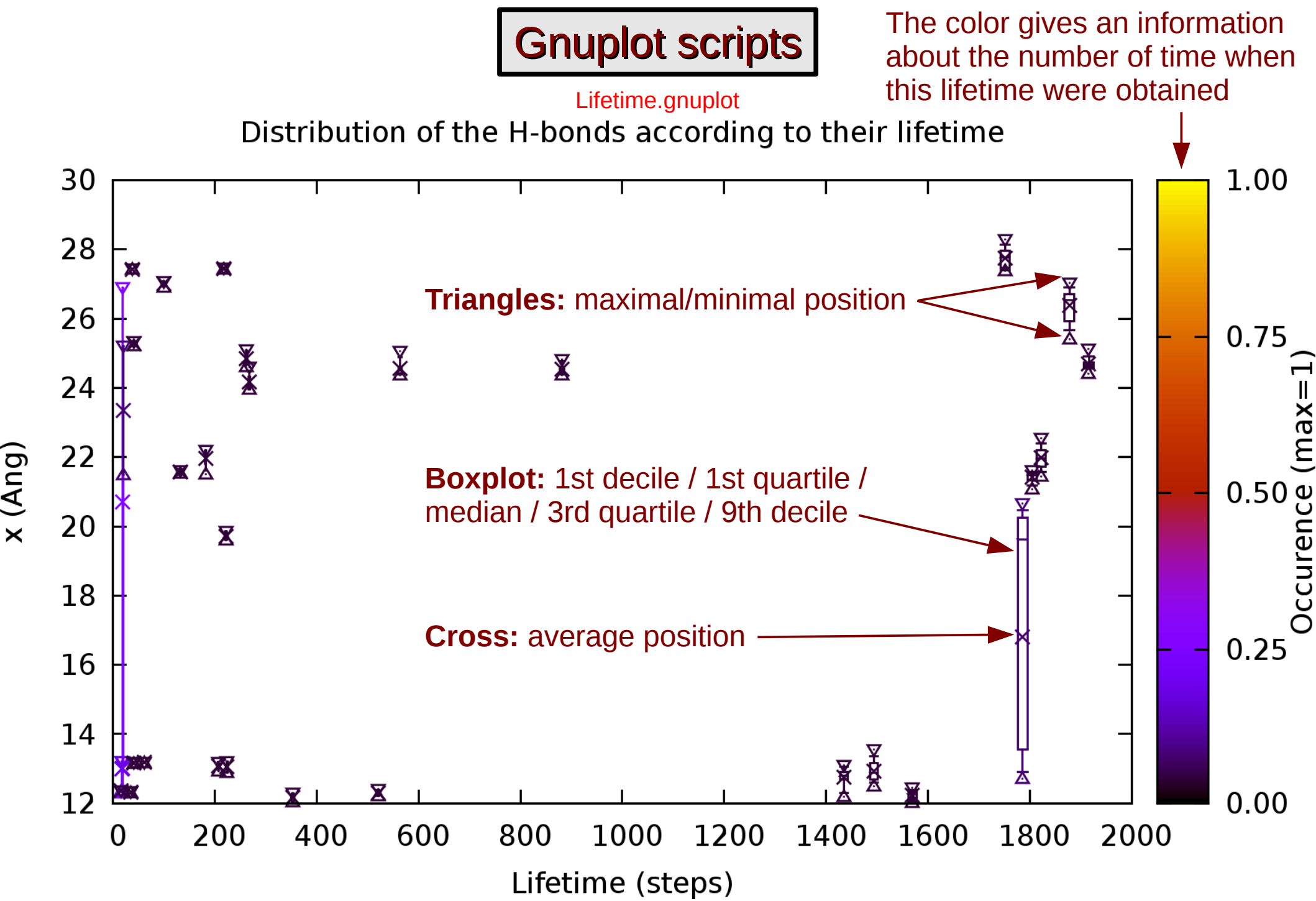
~/bin/__gnuplot/orientation_proj.sh 34 0.1 CaF2_H2O_neutral_xO.dat CaF2_H2O_neutral_vxH1.dat CaF2_H2O_neutral_vyH1.dat CaF2_H2O_neutral_vzH1.dat CaF2_H2O_neutral_vxH2.dat CaF2_H2O_neutral_vyH2.dat CaF2_H2O_neutral_vzH2.dat > orientation_proj.dat

~/bin/__gnuplot/angle.sh 34 11.59 13.38 0.1 CaF2_H2O_neutral_xO.dat CaF2_H2O_neutral_yO.dat CaF2_H2O_neutral_zO.dat CaF2_H2O_neutral_vxH1.dat CaF2_H2O_neutral_vyH1.dat CaF2_H2O_neutral_vzH1.dat CaF2_H2O_neutral_vxH2.dat CaF2_H2O_neutral_vyH2.dat CaF2_H2O_neutral_vzH2.dat > angle.dat

~/bin/__gnuplot/angle_proj.sh 34 0.1 CaF2_H2O_neutral_xO.dat CaF2_H2O_neutral_vxH1.dat CaF2_H2O_neutral_vyH1.dat CaF2_H2O_neutral_vzH1.dat CaF2_H2O_neutral_vxH2.dat CaF2_H2O_neutral_vyH2.dat CaF2_H2O_neutral_vzH2.dat > angle_proj.dat

Gnuplot scripts

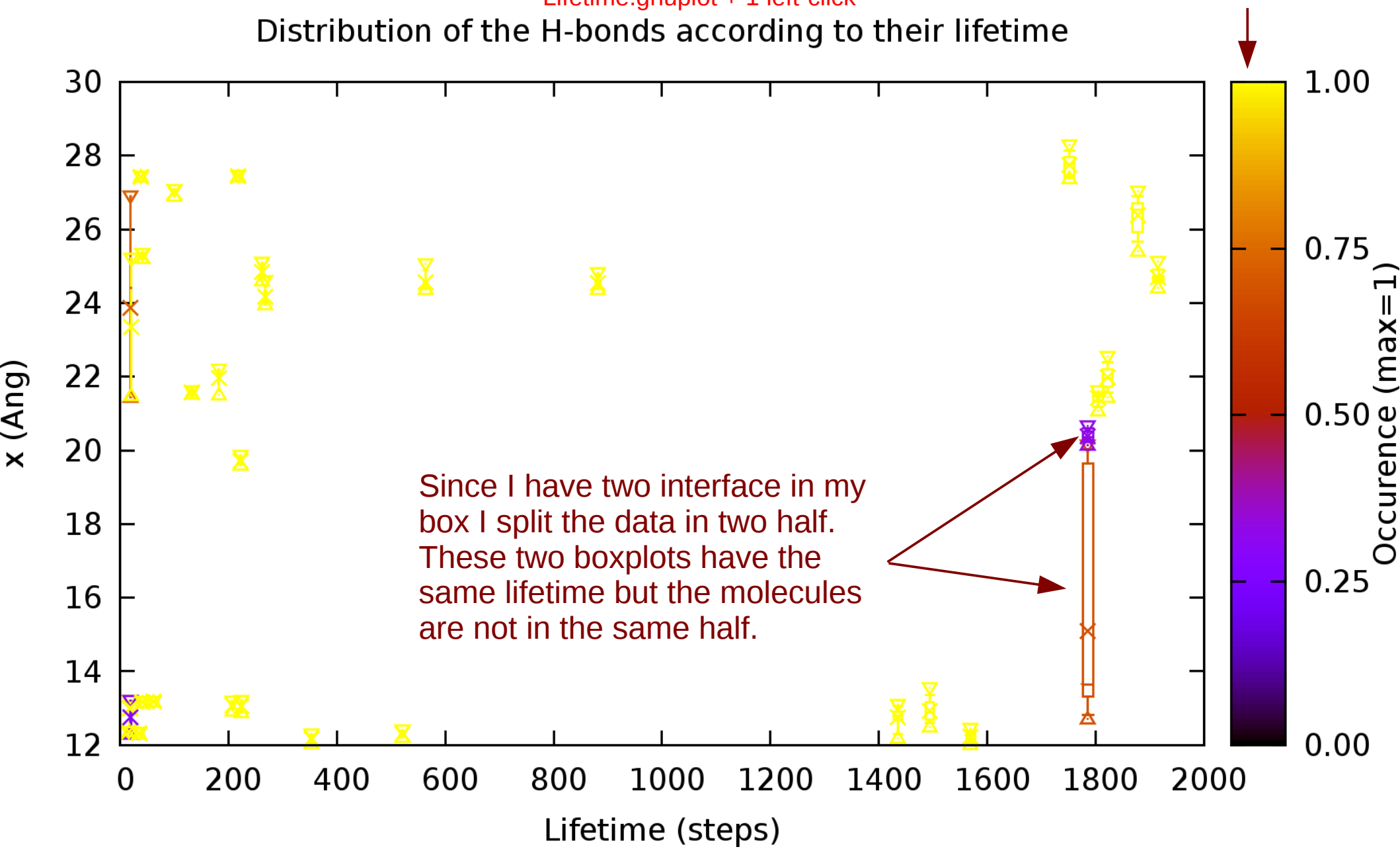
Lifetime.gnuplot



Gnuplot scripts

Lifetime.gnuplot + 1 left-click

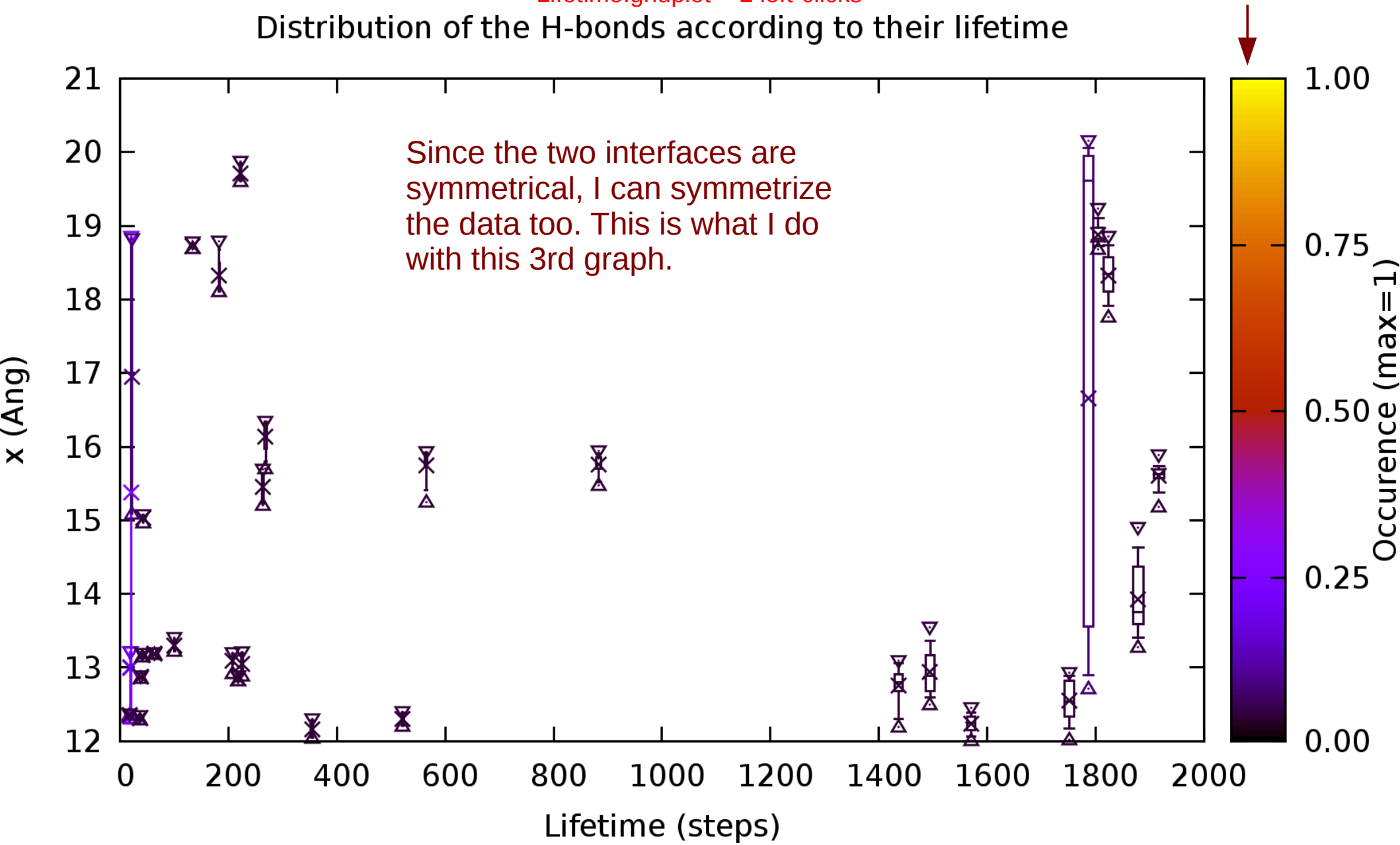
The color gives an information about the distribution of the molecules in the two half of the slab



Gnuplot scripts

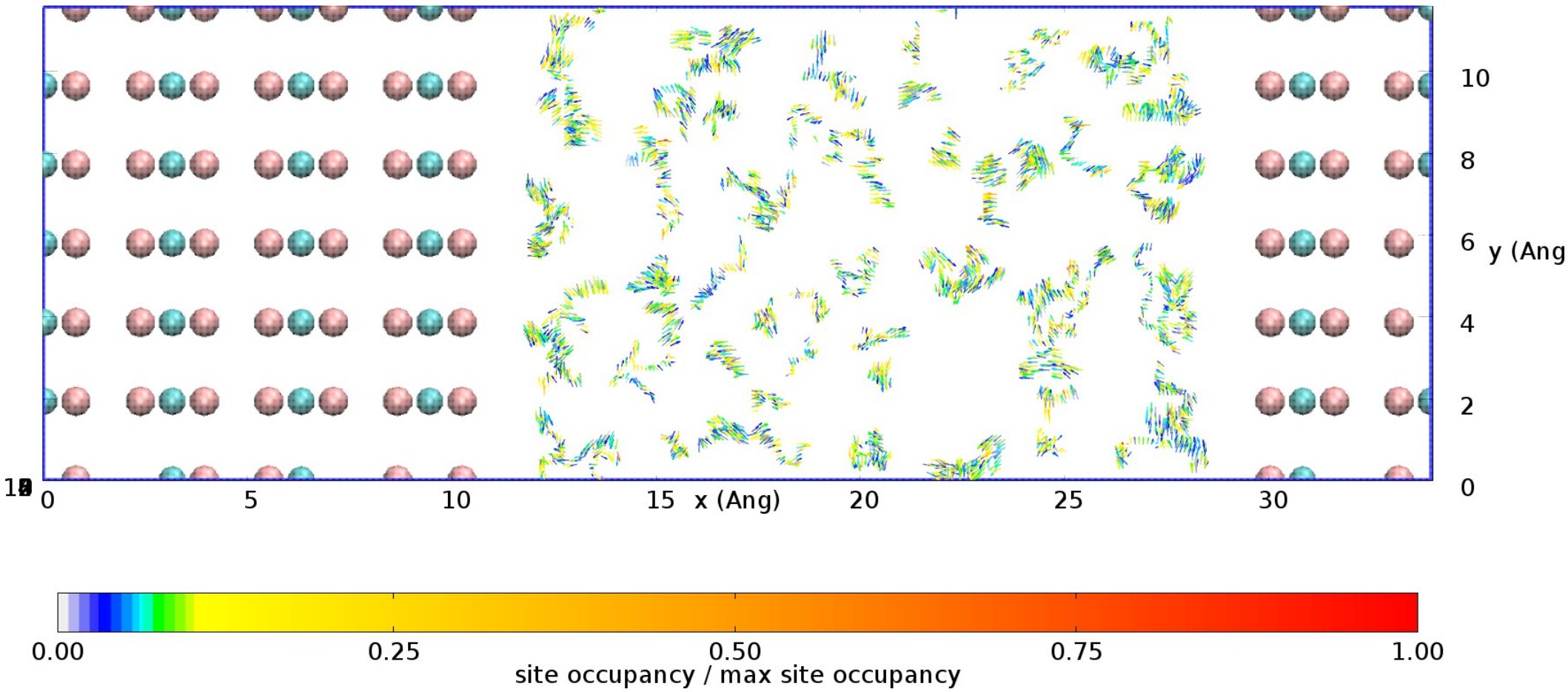
Lifetime.gnuplot + 2 left-clicks

Same meaning than for the first graph.



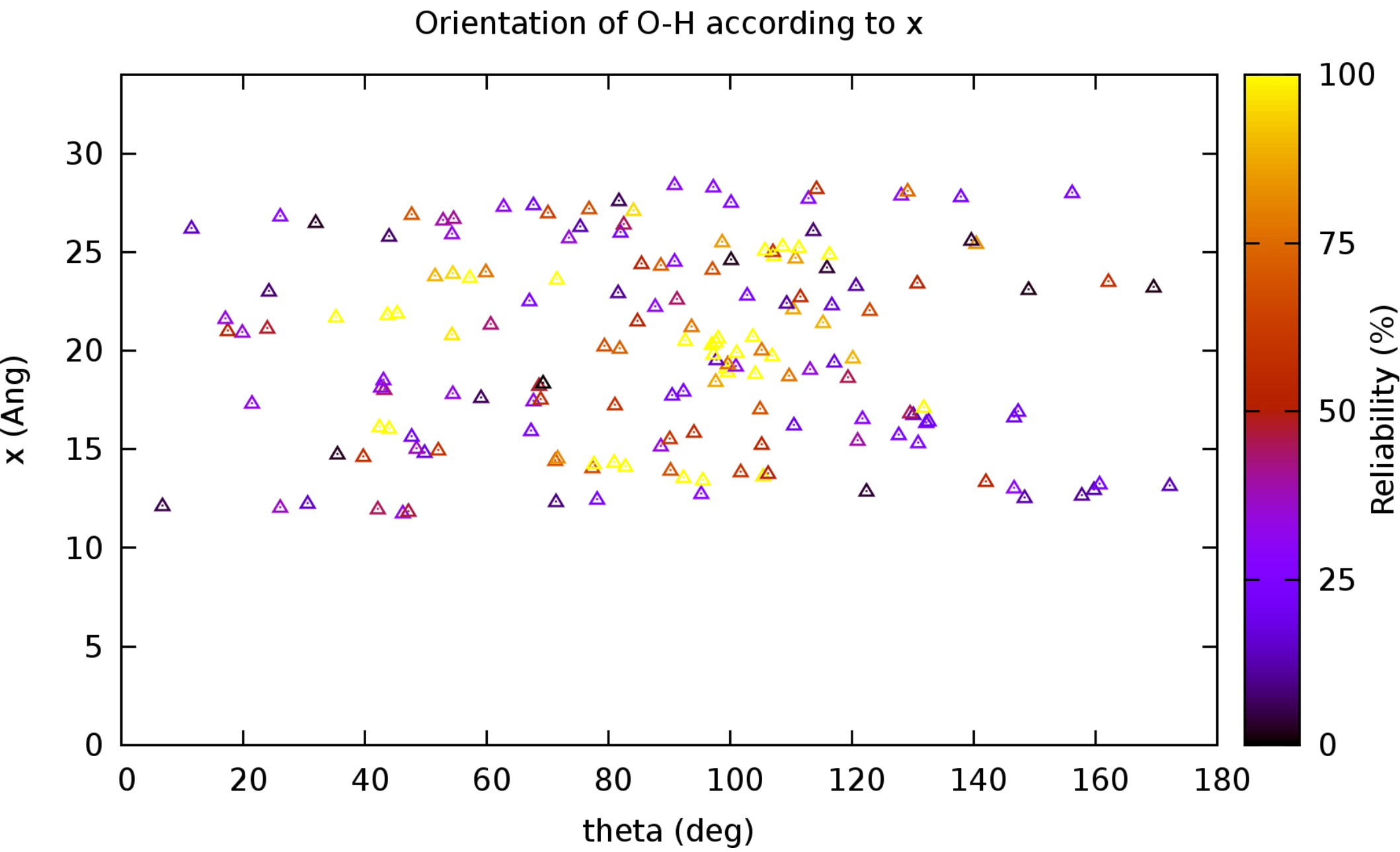
Gnuplot scripts

orientation.gnuplot



Average orientation over the time of MX2 according to x,y,z. It represents the dipole orientation. The color is associated with the time spent by the molecule in the region

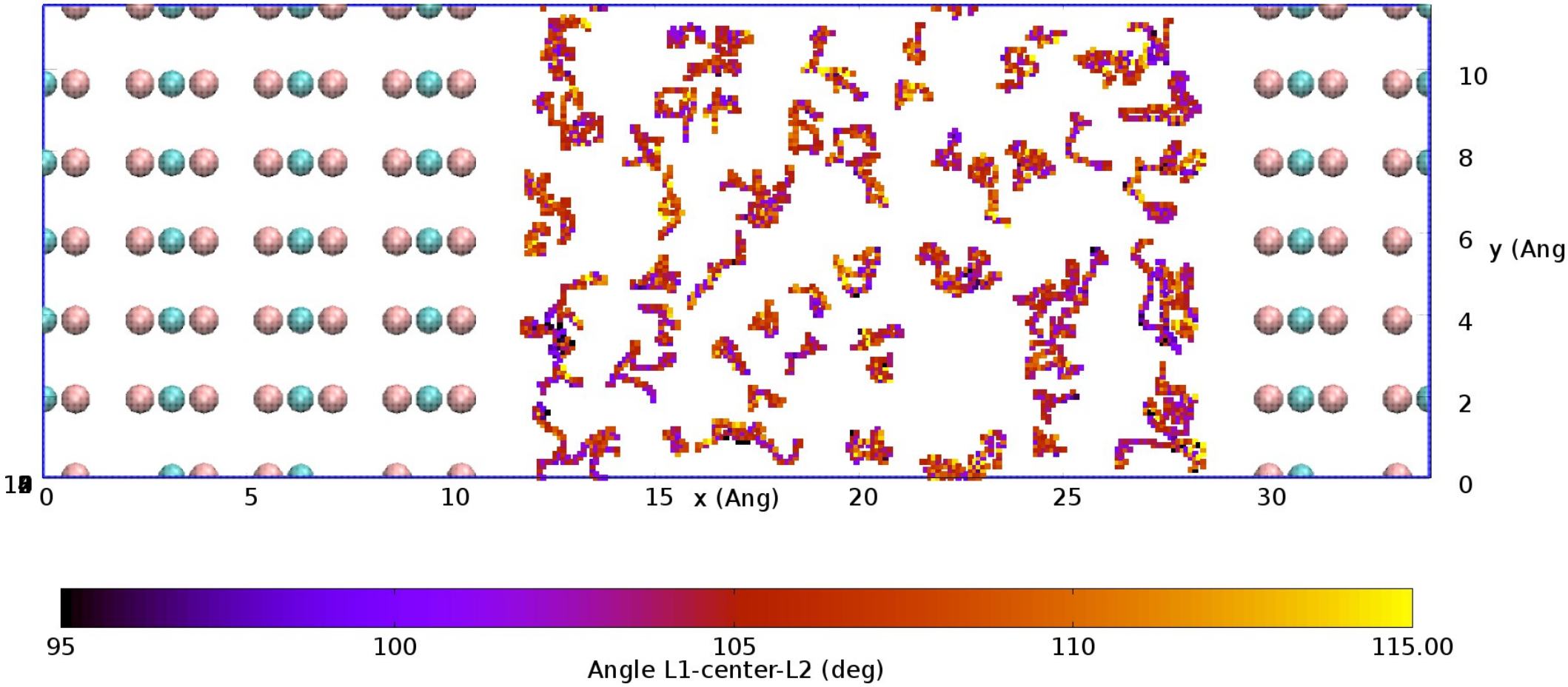
Gnuplot scripts



Average orientation over the time of MX2 according to x.

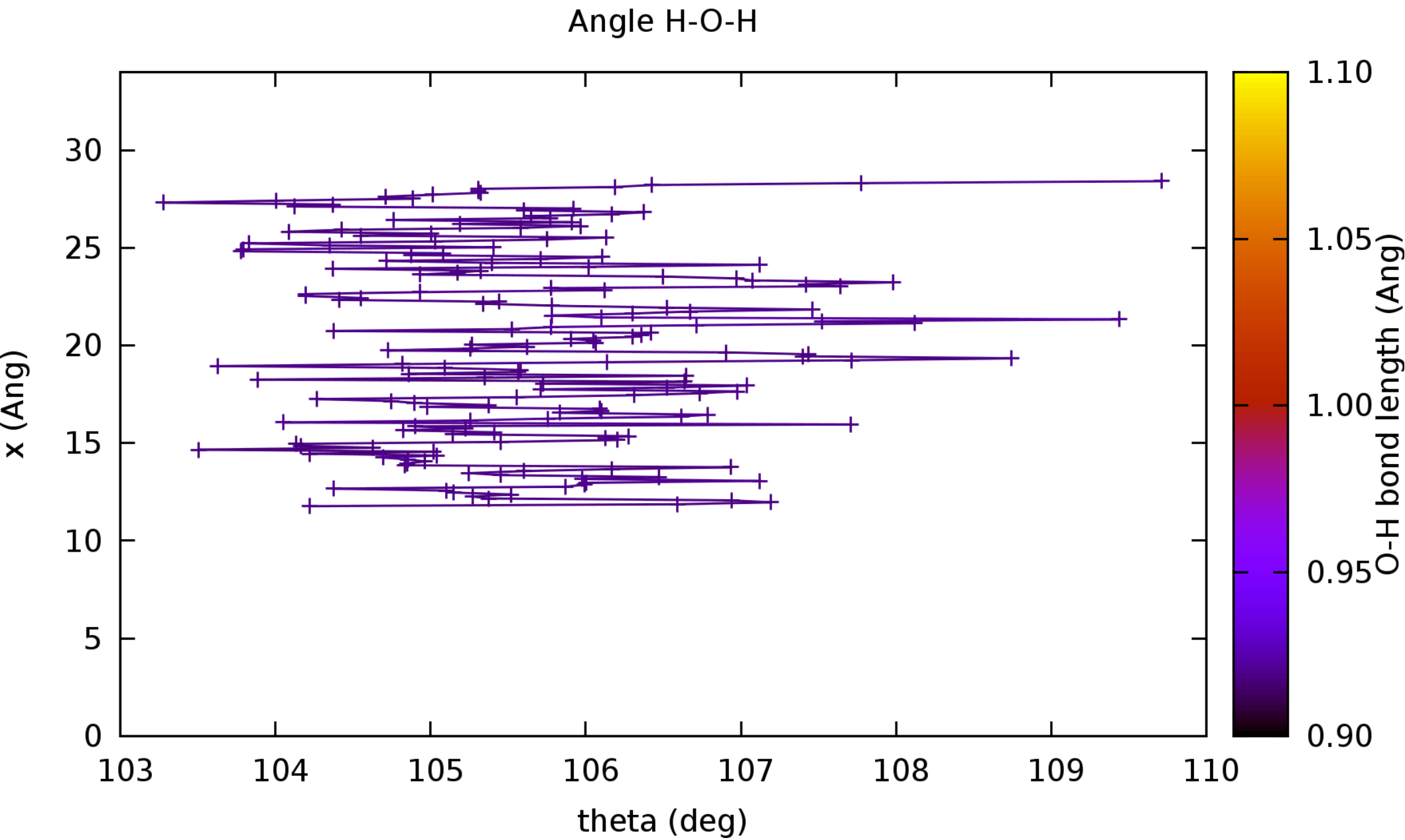
!!! The reliability factor has not yet a signification and will be certainly improved!!!

Gnuplot scripts



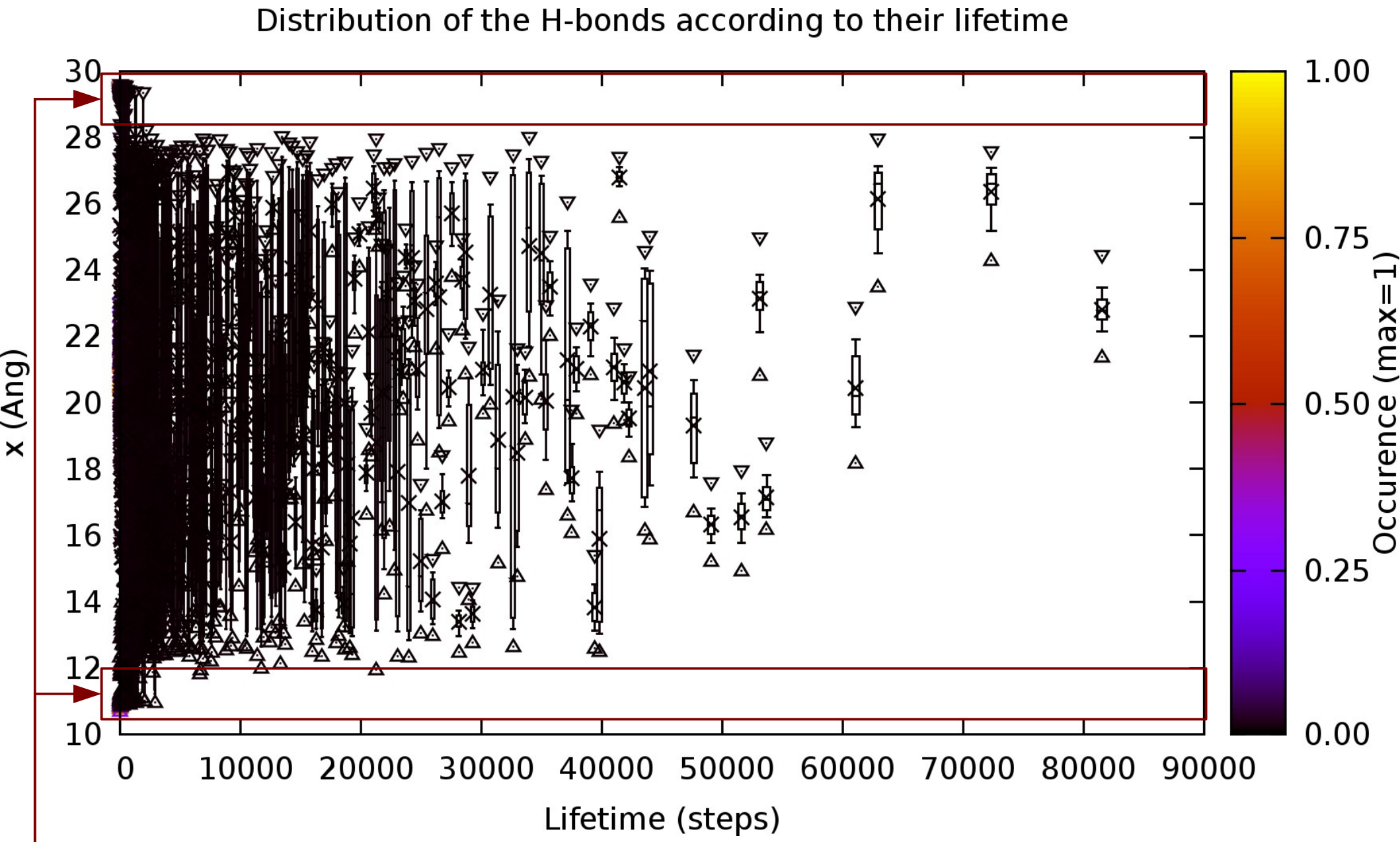
Average angle over the time of MX2 according to x,y,z. Especially useful for H-bond (O-H---O).

Gnuplot scripts

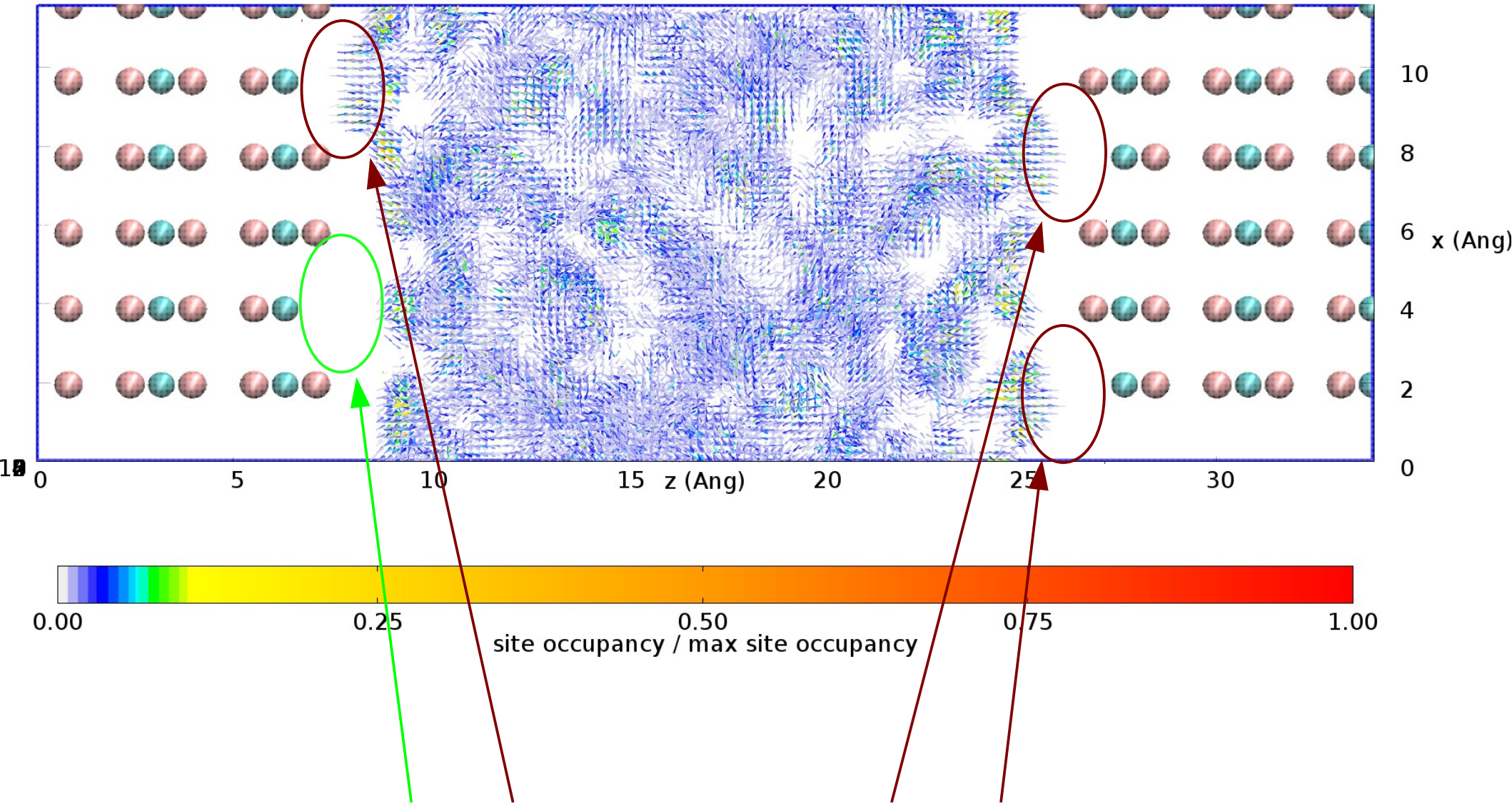


Average angle over the time of MX2 according to x. Especially useful for H-bond (O-H---O).

Real examples from my systems

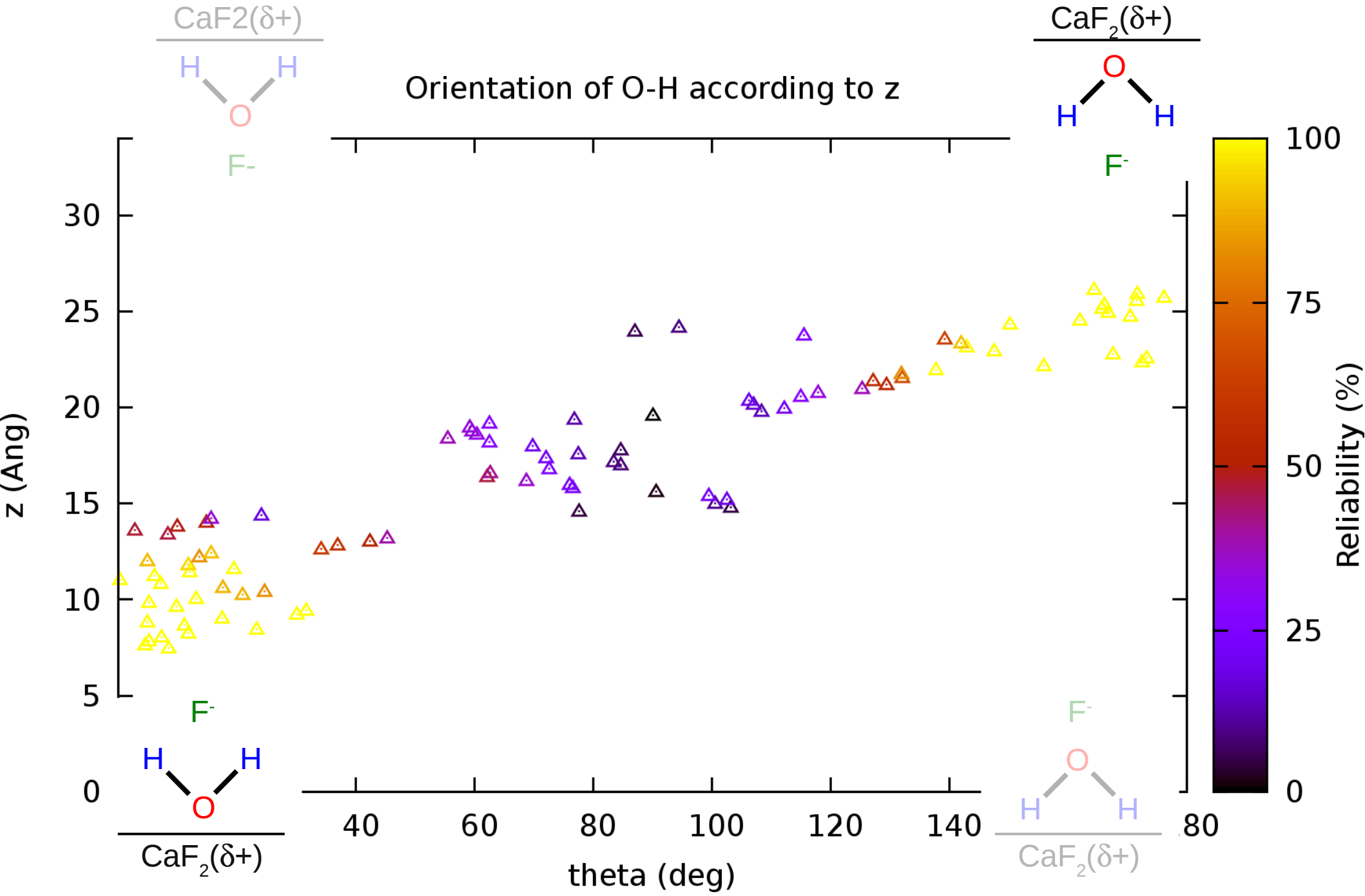


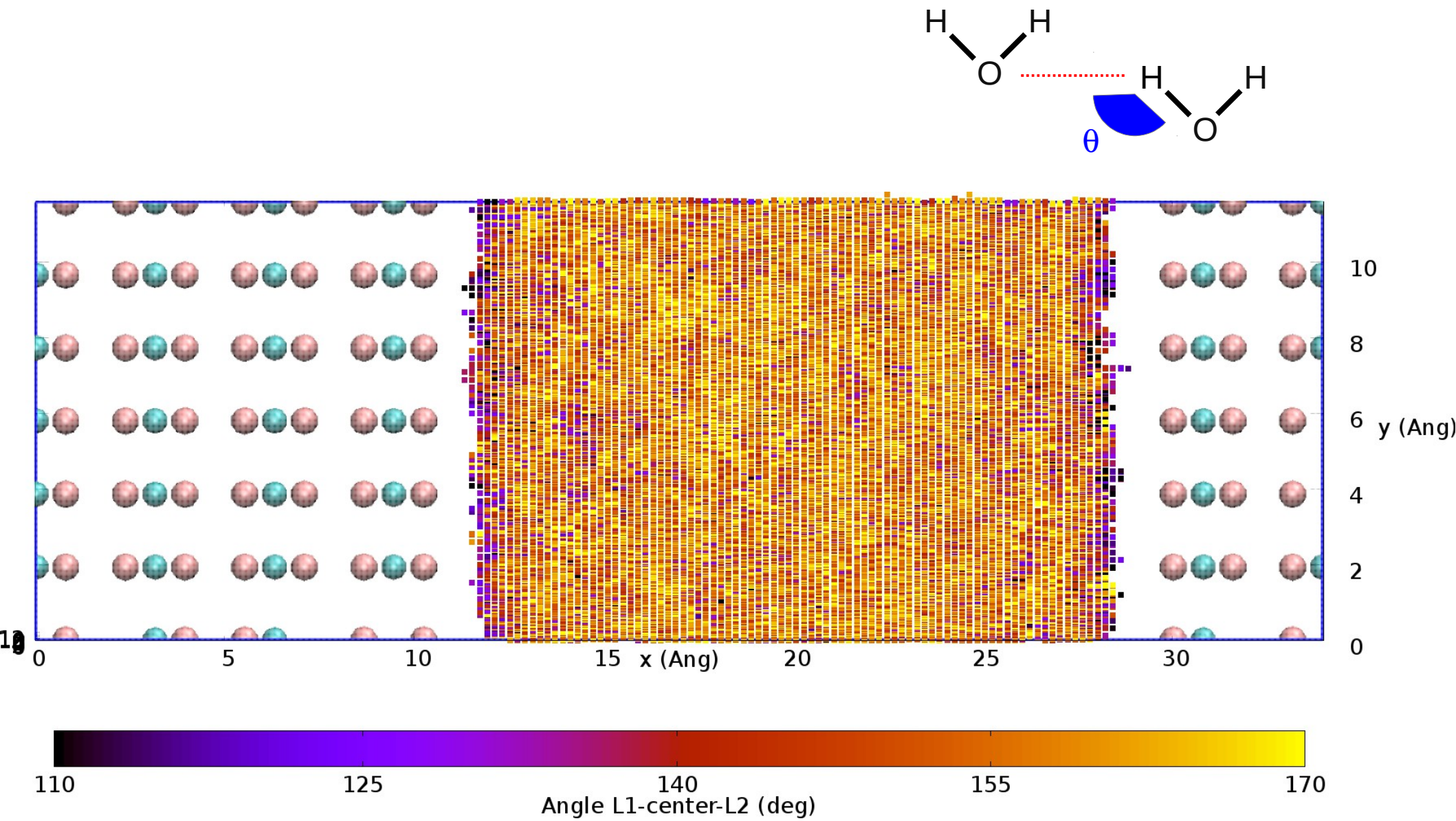
Here, I can see that at the interface, the lifetime of the water molecule is really short.



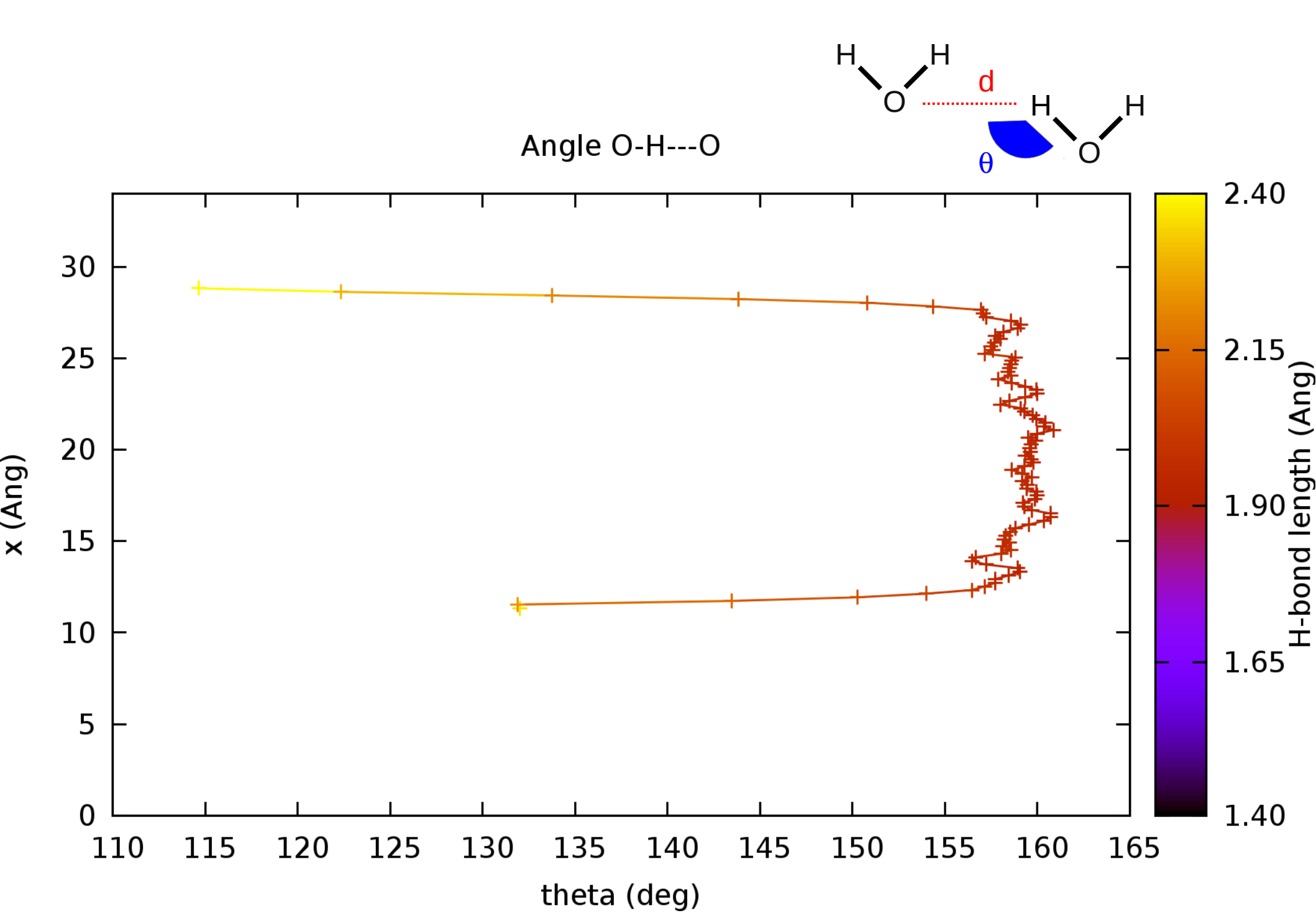
The water molecules fills 3 over 4 vacancies. Maybe because in the last one there is a O-H group

In this case, I can see that at the interface the dipole is oriented to the interface (and not to the bulk)





The angle between O-H---O is smaller at the interface (purple/black) than in the bulk (red/yellow).



Confirmation of the previous graph thanks to the length bond. The smaller angle, the weaker H-bond. So it is not surprising to see the length bond which increase at the interface.