

Auto-ionization of water

Trajectory Information:

- Software: LAMMPS
- Timestep: 0.5 fs
- Steps: 10,000
- Temperature: 300K
- Box Length: 46.937
- Force Field: NNP
- Ensemble: NVT
- Driven by a CV written in plumed
- System: 64 water molecules

pK_w calculations:

Object Attributes:

Following are the important attributes of the object Atom:

- x(float)
- y(float)
- z(float)
- element(string)
- hydrogens (list of tuples)
- oxygen (Atom object ref.)

Counting protons, OH- :

For 200 configurations:

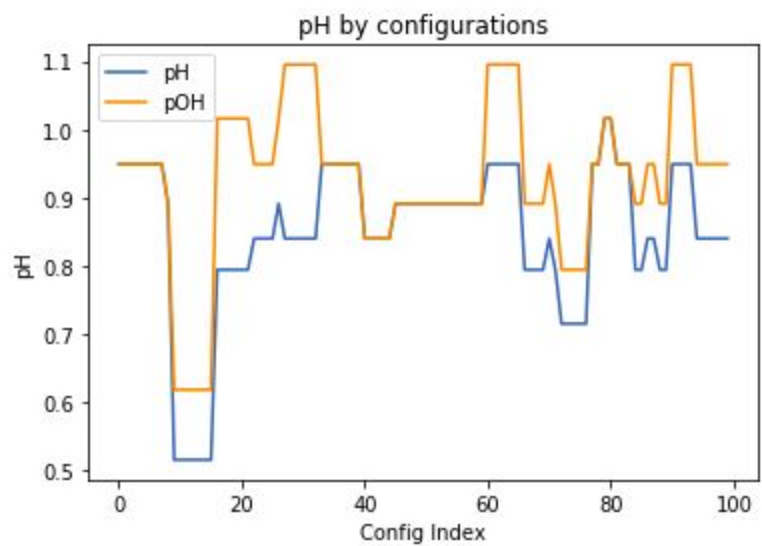
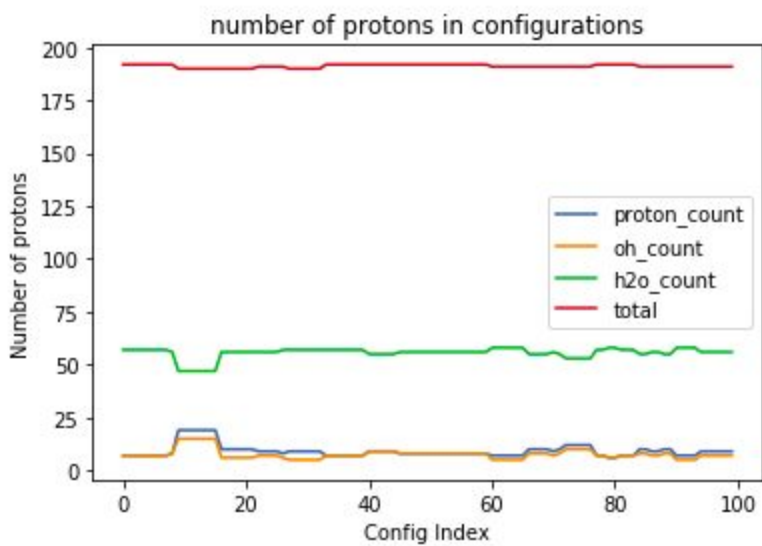
Algorithm:

```
for every O:
    for every H:
        If OH distance < cutoff :
            If len(O.hydrogens) < 2:
                O.hydrogen.add(H,distance)
                Sort (O.hydrogen by distance)
            else:
                O.hydrogen.pop()
                O.hydrogen.add(H,distance)
                Sort(O.hydrogen by distance)
```

Counting:

```
For every atom:
    If (H atom and no linked O):
        Proton_count++
    Else if (O atom and 1 linked H):
        OH_count++
    Else if (O atoms and 2 linked H):
        Water_count++
```

Results:



[Link to Code](#)

Some numbers: (Not corresponding by order)

H, OH-, H₂O, Total

number of atoms = 192

(10, 6, 56, 190)

number of atoms = 192

(10, 6, 56, 190)

number of atoms = 192

(10, 6, 56, 190)

number of atoms = 192

(9, 7, 56, 191)

number of atoms = 192

(9, 7, 56, 191)

number of atoms = 192

(9, 7, 56, 191)

number of atoms = 192

(9, 7, 56, 191)

number of atoms = 192

(8, 6, 57, 191)

number of atoms = 192

(9, 5, 57, 190)

number of atoms = 192

(9, 5, 57, 190)

number of atoms = 192

(9, 5, 57, 190)

number of atoms = 192

(9, 5, 57, 190)

number of atoms = 192

(9, 5, 57, 190)

number of atoms = 192

(9, 5, 57, 190)

number of atoms = 192

(7, 7, 57, 192)

number of atoms = 192

(7, 7, 57, 192)

number of atoms = 192

(7, 7, 57, 192)

number of atoms = 192

(7, 7, 57, 192)

number of atoms = 192

(7, 7, 57, 192)

number of atoms = 192

pH,pOH by config=

[illegible]

pKw by config=

[illegible]

1.8104425426843704
1.8104425426843704
1.8104425426843704
1.8104425426843704
1.7892532436144322
1.7892532436144322
1.7892532436144322
1.7892532436144322
1.9073525556924267