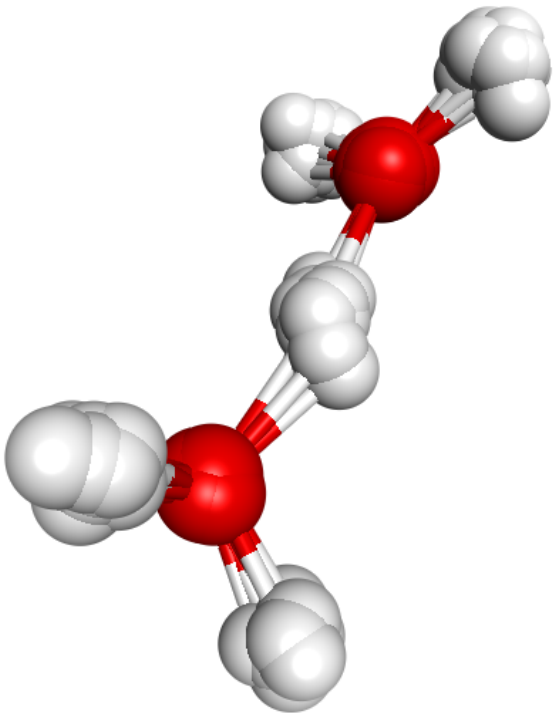
Path integral molecular dynamics (PIMD)

1. Calculation setup

The following setup is used.

- Method : PIMD
- Ensemble : NVT (canonical ensemble)
- Potential : SMASH (b3lyp/cc-pvdz)
- Number of beads : 16
- Boundary : free boundary condition
- System : protonated water dimer

A snapshot is shown below.



2. Results

As shown below, the total energy, the potential energy, the instantaneous temperature and the wall clock time of each step are printed in “standard.out”.

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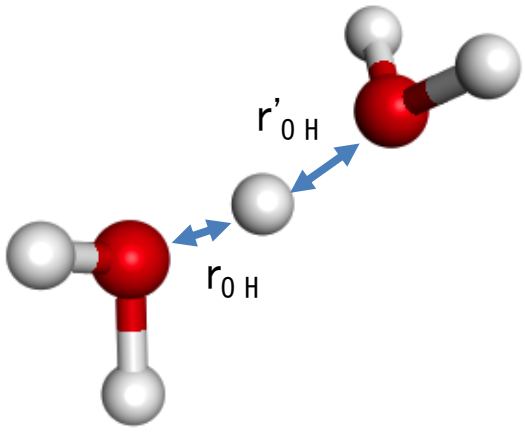
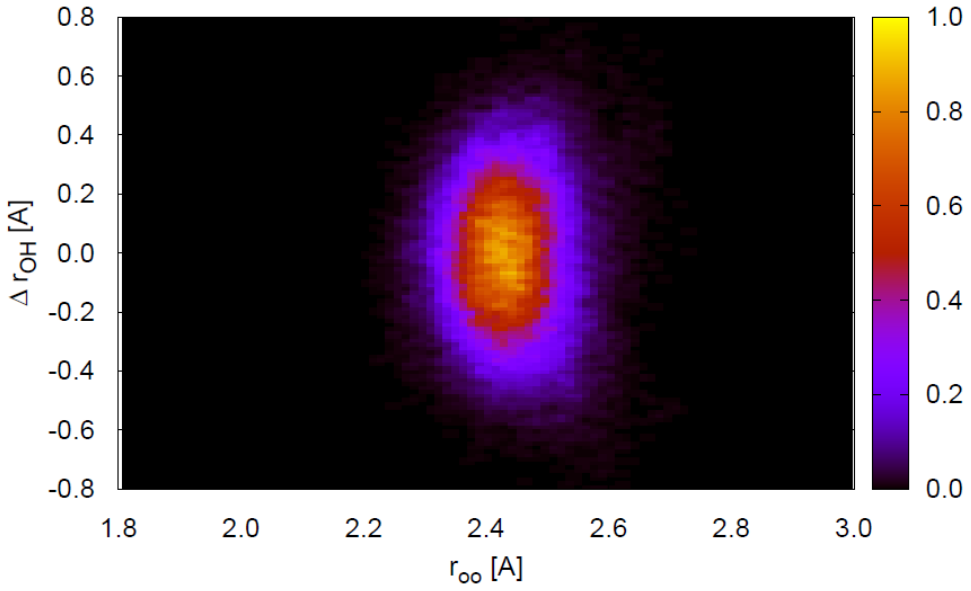
================================================================================
   step     energy [au]  potential [au]  temp [K]  wall clock time
--------------------------------------------------------------------------------
      0   -152.18893397   -153.07017355    300.00  2016-04-25 月 09:12:32.28
      1   -152.18894445   -153.07123665    302.08  2016-04-25 月 09:12:55.69
      2   -152.18896233   -153.07337533    307.25  2016-04-25 月 09:13:18.87
      3   -152.18898309   -153.07630145    314.45  2016-04-25 月 09:13:42.26
      4   -152.18900223   -153.07961072    320.76  2016-04-25 月 09:14:05.64
      5   -152.18901748   -153.08290248    324.19  2016-04-25 月 09:14:29.18
      6   -152.18902891   -153.08590948    325.73  2016-04-25 月 09:14:52.62
      7   -152.18903723   -153.08851938    326.82  2016-04-25 月 09:15:15.31
      8   -152.18904302   -153.09070411    327.54  2016-04-25 月 09:15:38.60
      9   -152.18904660   -153.09245733    327.80  2016-04-25 月 09:16:01.40
     10   -152.18904804   -153.09377275    327.60  2016-04-25 月 09:16:24.70
...omitted...
```

The figure in the next page is the hydrogen bond fluctuation shown as the two-dimensional distribution with respect to the vertical axis Δr_{OH} (see below figure) and the horizontal axis r_{OO}.

$$\Delta r_{OH} = r_{OH} - r'_{OH}$$




0.8
0.6
0.4
0.2
0.0
-0.2
-0.4
-0.6
-0.8
Δ r_OH [A]
1.8
2.0
2.2
2.4
2.6
2.8
3.0
r_oo [A]
1.0
0.8
0.6
0.4
0.2
0.0