QXMD Hands-on Session

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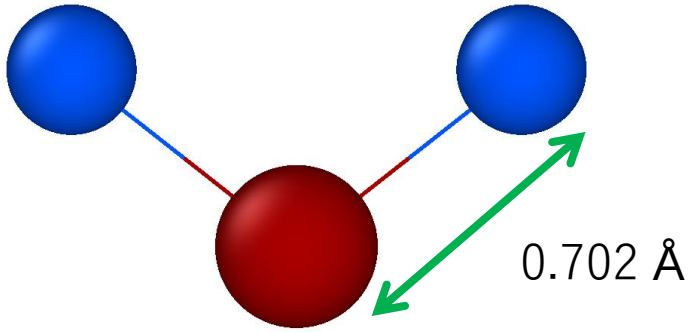
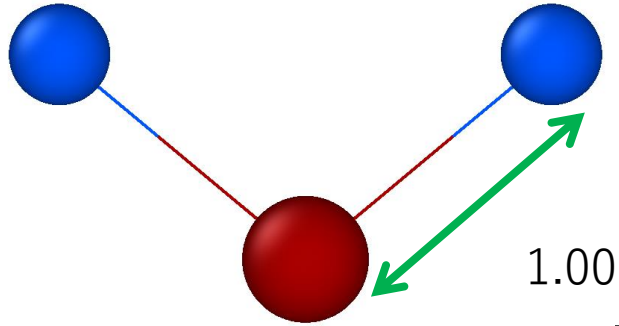
Outline for QXMD Hands-on

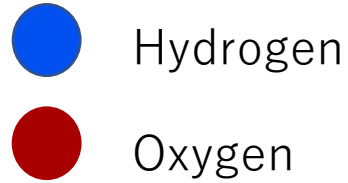
1. Optimize Water Structure
2. Adiabatic Quantum Molecular Dynamics (QMD)
3. Non-adiabatic Quantum Molecular Dynamics (NAQMD)

1. Optimize Water Structure

- **We will use QXMD to optimize water molecule**

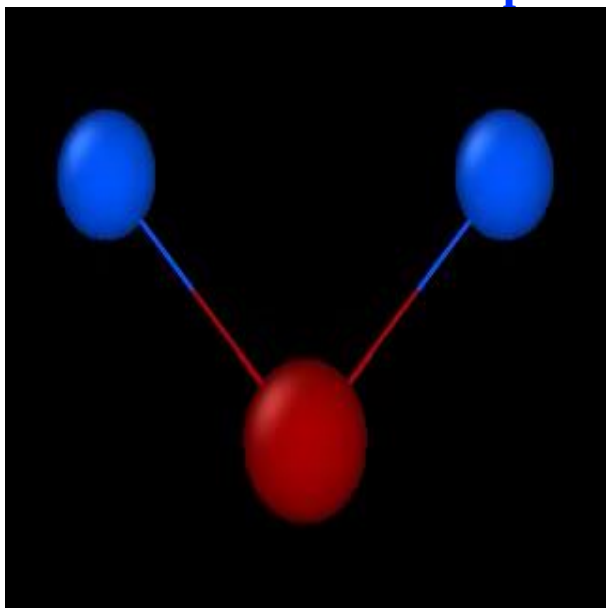


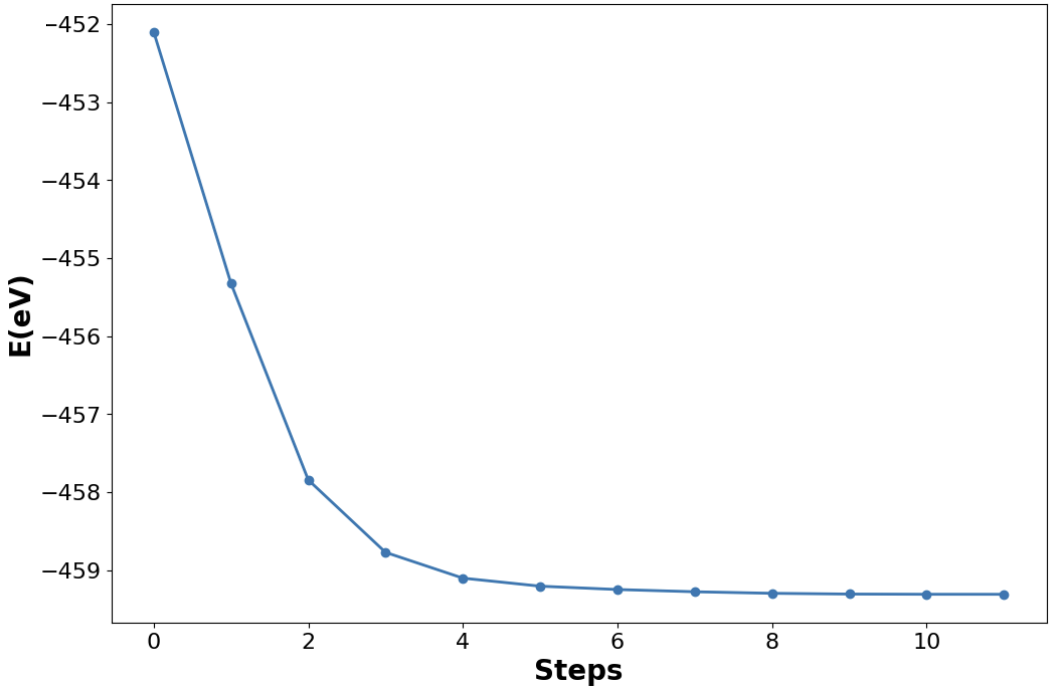




Initial Structure

Optimized Structure





Energy Convergence

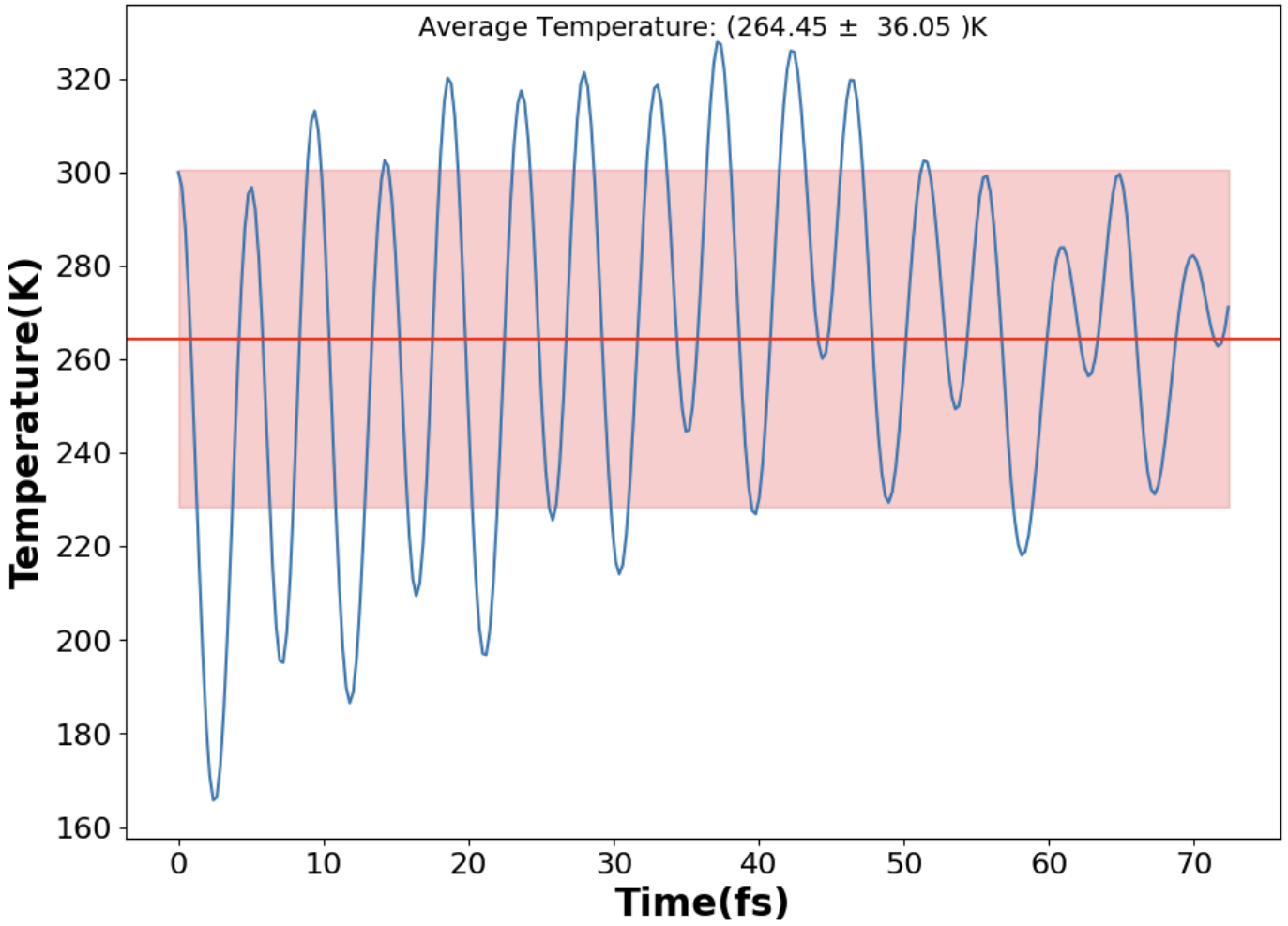
1.Optimization Input File

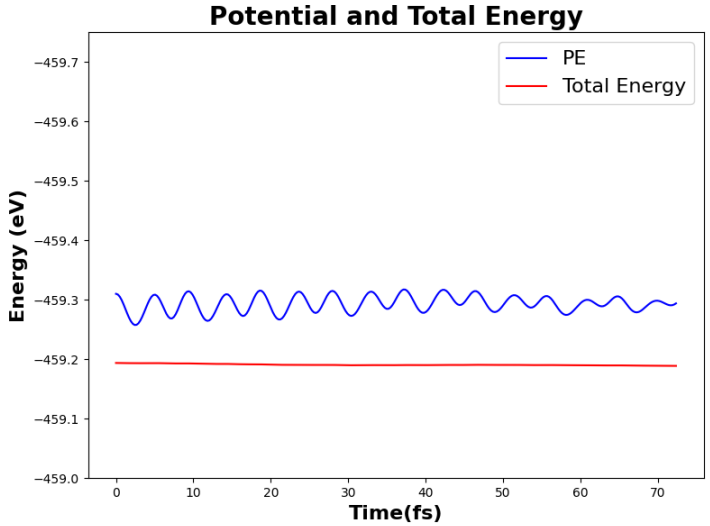
IN.PARAM

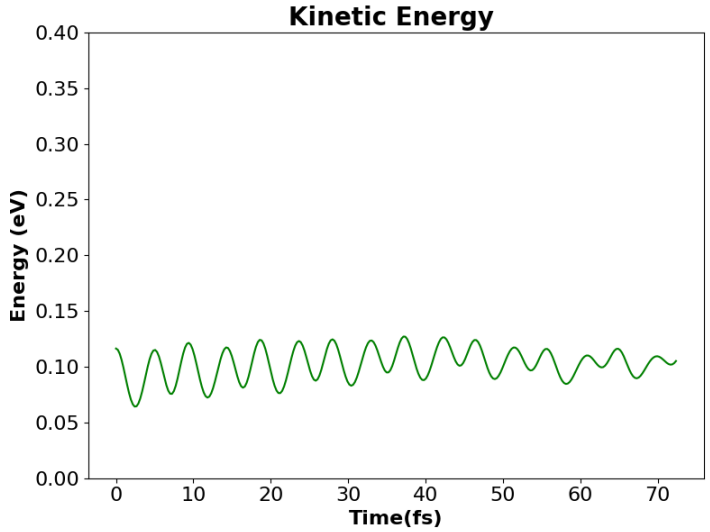
```
*molecular dynamics              :
(method)                         :
   1                             : (ifmd)
                                 :   0:non, 1:optimization, 2:NVE, 3:NVT, 4:NPT
(time step)                      :
   0.1d0   100                   : (dtmd, nstop) time step, total step
                                 :
(optimization)                   : only for structural optimization (ifmd == 1 )
   2                             : (ioptmze)
                                 :  -1: do not optimize atomic coordinates
                                 :   0: Conjugate gradient
                                 :   1: Projected velocity Verlet
                                 :   2: Quasi-Newton method with BFGS formula
(output data)                    : only for MD nodes
    1                            : (ioskip)  skip step
 .true.                          : (locoor) .true. = output scaled coordinates
 .true.                          : (lovelo) .true. = output scaled velocities
 .true.                          : (loforc) .true. = output scaled forces
                                 :
(tolerance)                      : tolerance for CG optimization (ifmd == 1 )
  1.d-07                         : (tol_energy) energy/atom in [a.u.]
  5.d-04                         : (tol_force ) max. force  in [a.u.]
                                 :
*end                             :
```

2. Adiabatic Quantum Molecular Dynamics (QMD)

- **We will run a QMD simulation in NVE ensemble for the water molecule**







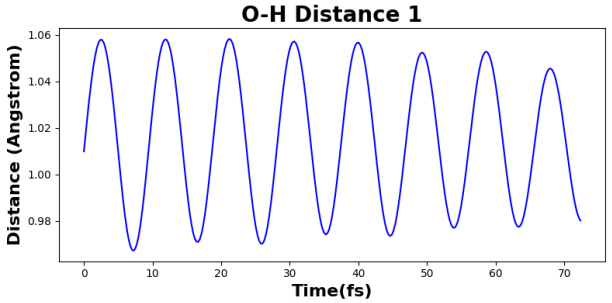
2.QMD Input File

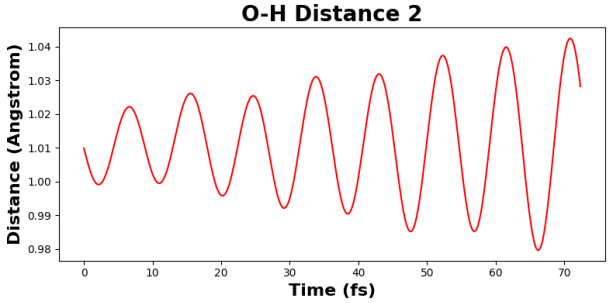
IN.PARAM

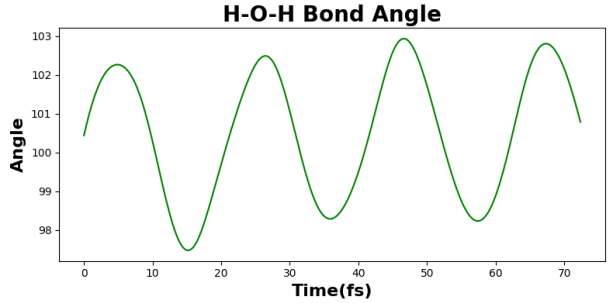
```
*molecular dynamics            :
(method)                       :
   2                           : (ifmd)
                               :   0:non, 1:optimization, 2:NVE, 3:NVT, 4:NPT
(time step)                    :
   10.0d0  300                 : (dtmd, nstop) time step, total step
(temperature)                  : only for real dynamics (NVE-, NVT-, NPT-MD )
   300.d0                      : (treq) temperature in [K]
(check temperature)            :
  .false.                      : (liscale) .true. = Do it !
   25                          : (iscnum)  number of temperature check
   20                          : (iscstp)  skip step
                               :
(output data)                  : only for MD nodes
    1                          : (ioskip)  skip step
 .true.                        : (locoor) .true. = output scaled coordinates
 .true.                        : (lovelo) .true. = output scaled velocities
 .true.                        : (loforc) .true. = output scaled forces
                               :
*end                           :
```

3. Non-adiabatic Quantum Molecular Dynamics (NAQMD)

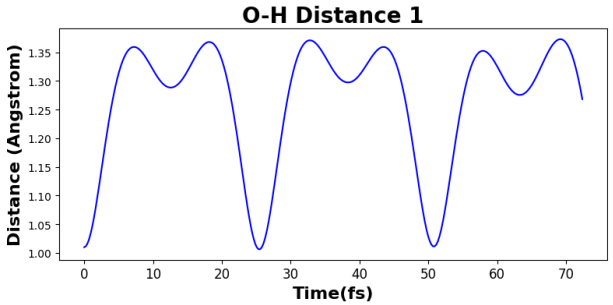
- **We will perform excited state dynamics with an electron and hole pair excited in the water molecule and evaluate bond length and bond angle.**

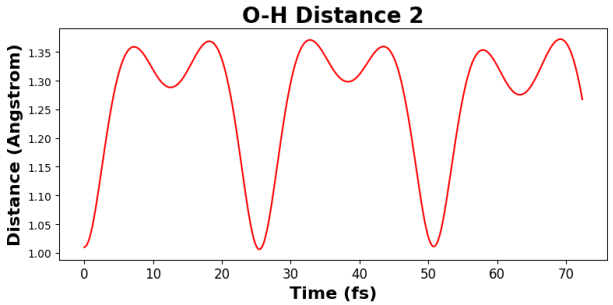


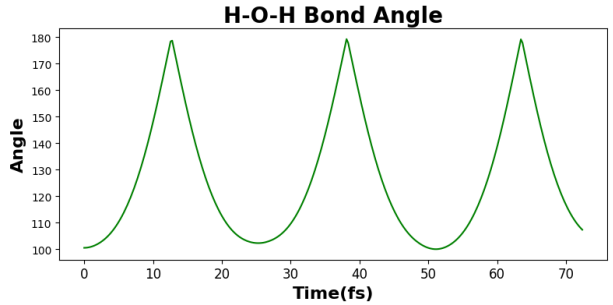




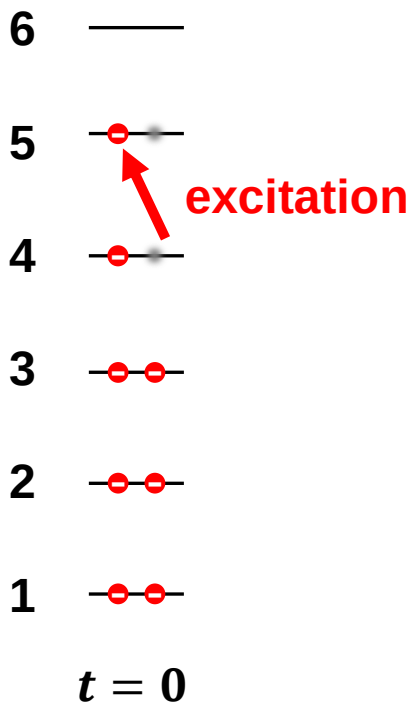
QMD Simulation







NAQMD Simulation



3.NAQMD Input File

IN.PARAM

```
*TDDFT-MD                        :
(how of it)                      :
 .true.                          : (ltddft) .true. = execute MD based on TDDFT
                                 :
(FSSH)                           :
 .true.                          : (ltddft_fssh) .true. = FSSH, .false. = Ehrenfest
                                 :
(FSSH-ground-state-SCF)          :
 .true.                          : (lfssh_gsscf) .true.  = SCF with the ground  state
                                 :               .false. = SCF with the excited state
(FSSH-mixing charge)             : only for lfssh_gsscf = .true.
   0.8d0  0.13d0                 : (aslh_fssh, bslh_fssh)
                                 :
(time step)                      :
   0.04d0                        : (dttddft) time step in [Hartree a.u.] in TDDFT-FSSH
                                 :
(restart)                        :
 .false.                         : (ltddft_start) .true. = restart
                                 :
(FSSH-random-initialize)         :
 .true.                          : (lfssh_random) .true. = manual, .false. = automatic
 1119041003.0000000              : (rseed_fssh) only for lfssh_random = .true.
(occupations)                    :
   2                             : (nocc_change) # of occupations to be changed
   4   1.0  0.0 → Hole           : (numband, occ_new) band index, occupations(up&down)
   5   1.0  0.0 → Electron       : (numband, occ_new) band index, occupations(up&down)
                                 :
*end                             :
```