QXMD Hands-on Session

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Collaboratory for Advanced Computing & Simulations

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CyberMAGICS Workshop

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Outline for QXMD Hands-on

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

Open Your Google Colab:
colab.research.google.com

F. Shimojo et al., SoftwareX 10, 100307 (2019).

1. Build QXMD

qxmdmpi
data/
control/ **NCPP**
CONFIG
filename
IN.PARAM: *parallel
*start
*approximation for Exc
*SCF iterations
*molecular dynamics
*supercell
*electronic bands
*dump wavefunctions
*atoms
……

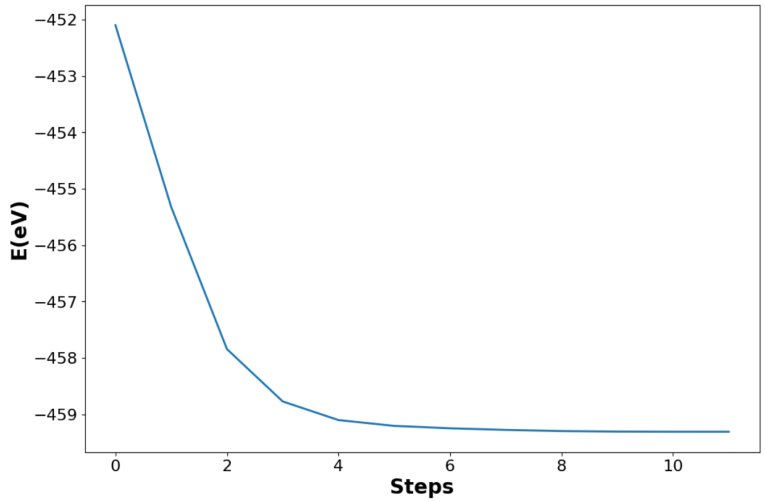
IN.VELOC

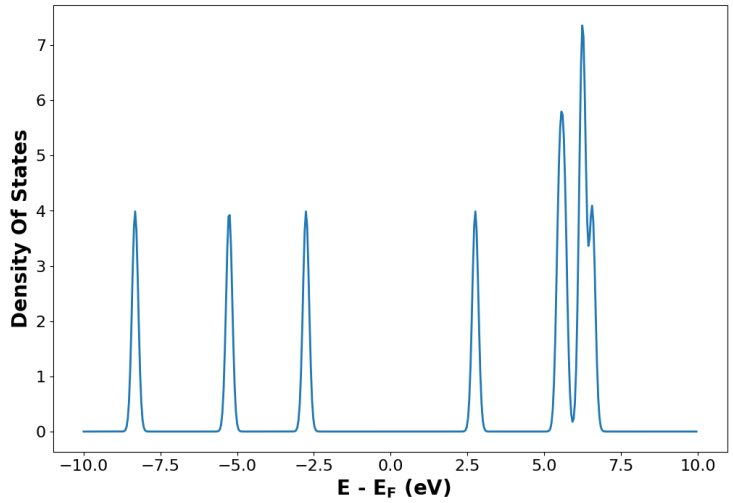
The manual for QXMD can be found at: https://usccacs.github.io/QXMD_DEV/

2. Optimize Water Structure

*molecular dynamics

ifmd: 1
dtmd: 0.1d0
nstop: 100
ioptmze: -1: do not optimize atomic coordinates
0: Conjugate gradient
1: Projected velocity Verlet
2: Quasi-Newton method with BFGS formula
tol_energy: 1.d-07
tol_force: 5.d-04



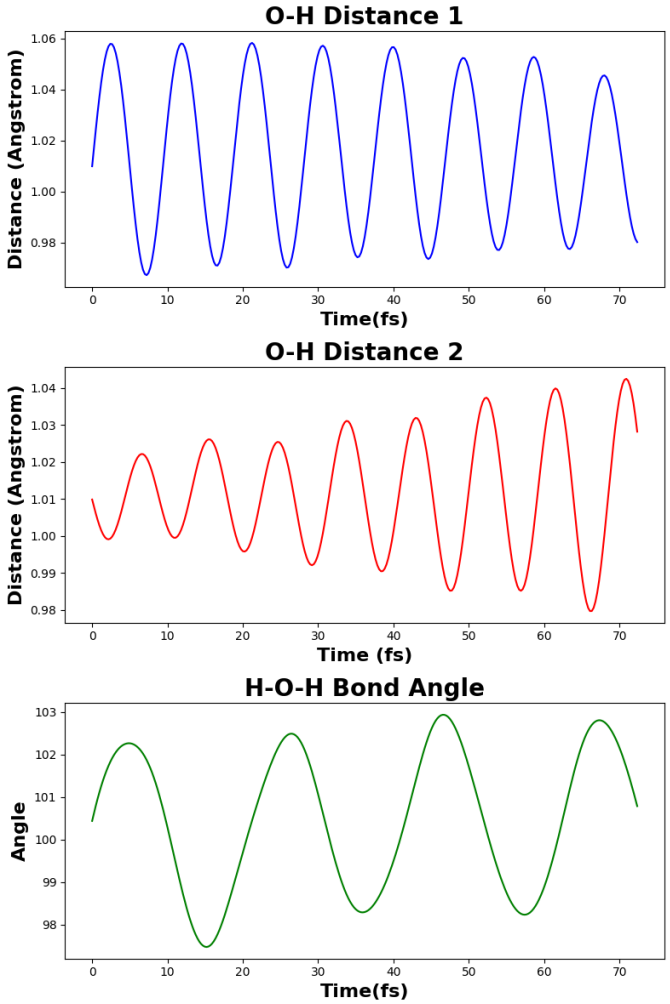


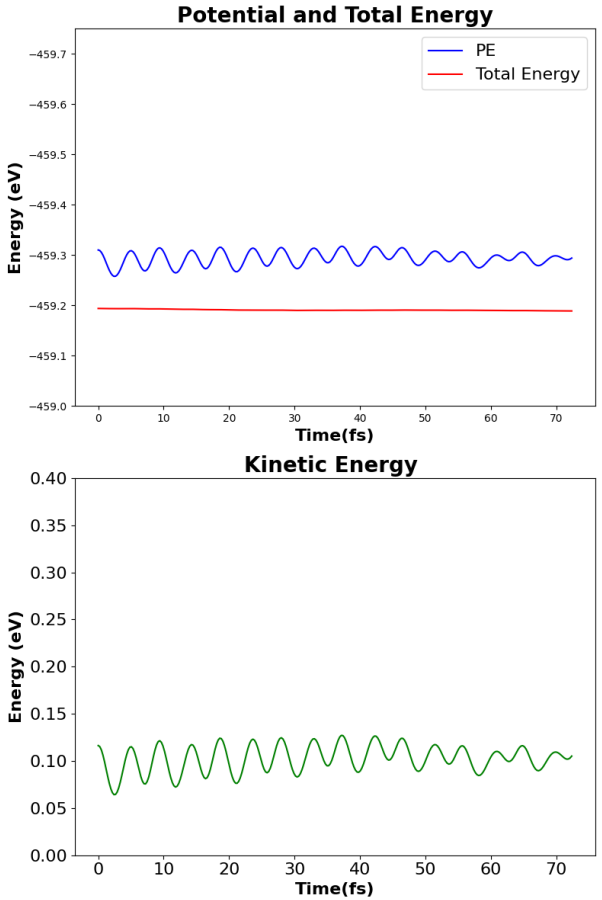
3. Adiabatic Quantum Molecular Dynamics (QMD)

*molecular dynamics

ifmd: 2:NVE
3:NVT
4:NPT

dtmd: 10.0d0
nstop: 300
treq: 300
ioskip: 1
locoor: .true.
lovelo: .true.
loforc: .true.





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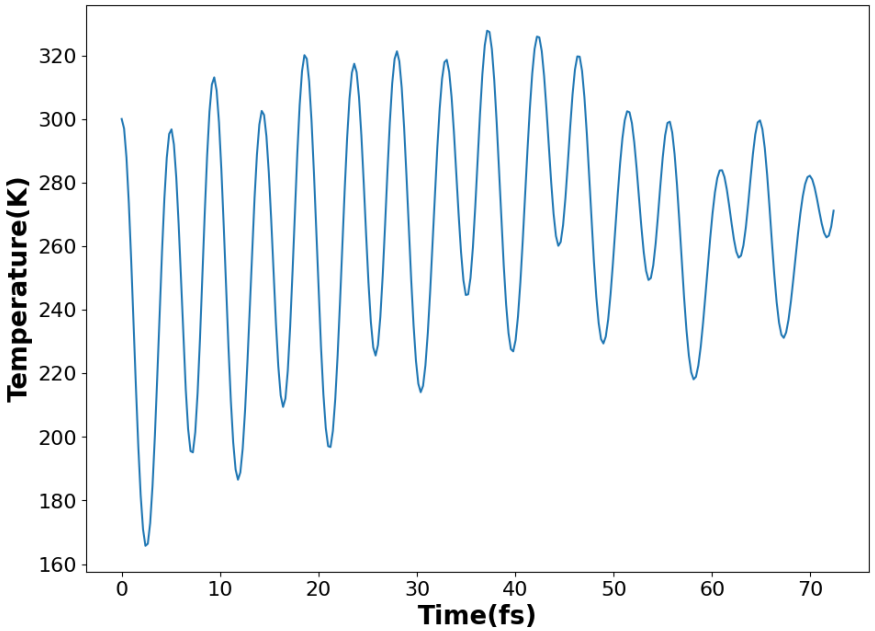
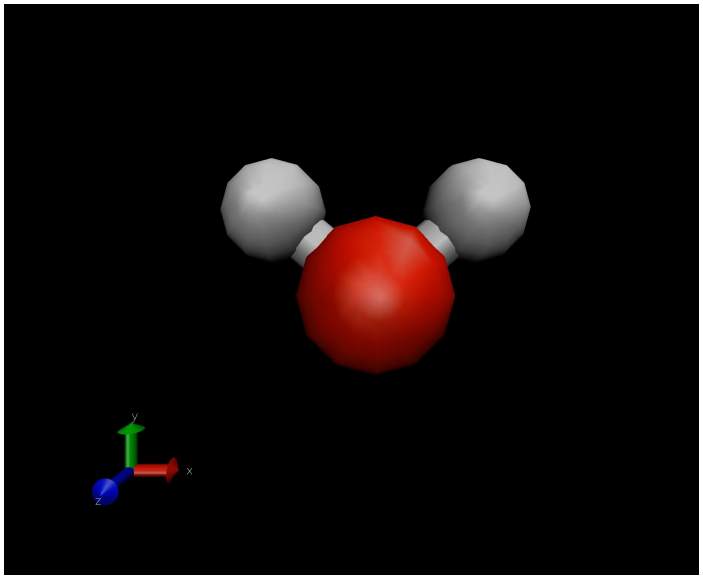


Trajectory Visualization



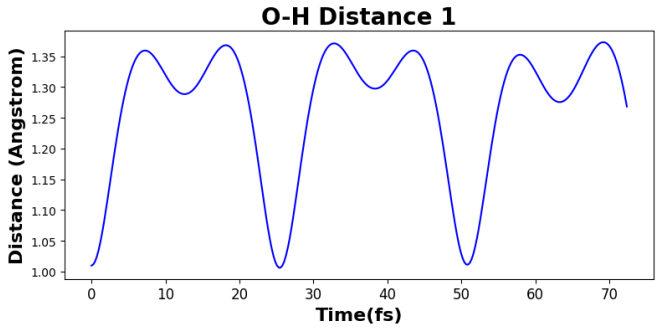
4. Non-adiabatic Quantum Molecular Dynamics (NAQMD)

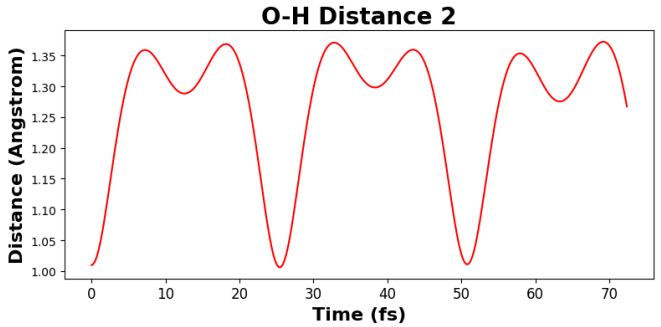
*molecular dynamics

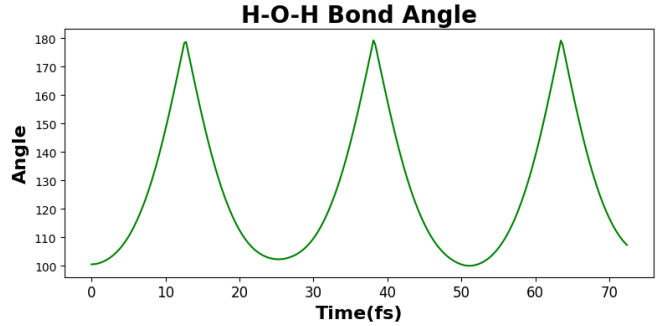
ifmd: 2
dtmd: 10.0d0
nstop: 300
treq: 0.1d0
ioskip: 1
locoor: .true.
lovelo: .true.
loforc: .true.

*TDDFT-MD

ltddft: .true.
ltddft_fssh : .true.
lfssh_gsscf: .true.
aslh_fssh: 0.8d0
bslh_fssh: 0.13d0
dttddft: 0.04d0
ltddft_start: .false.
lfssh_random: .true.
rseed_fssh:1119041003.0000000
nocc_change: 2
numband: 4
occ_new: 1.0 0.0

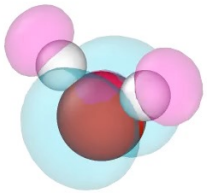




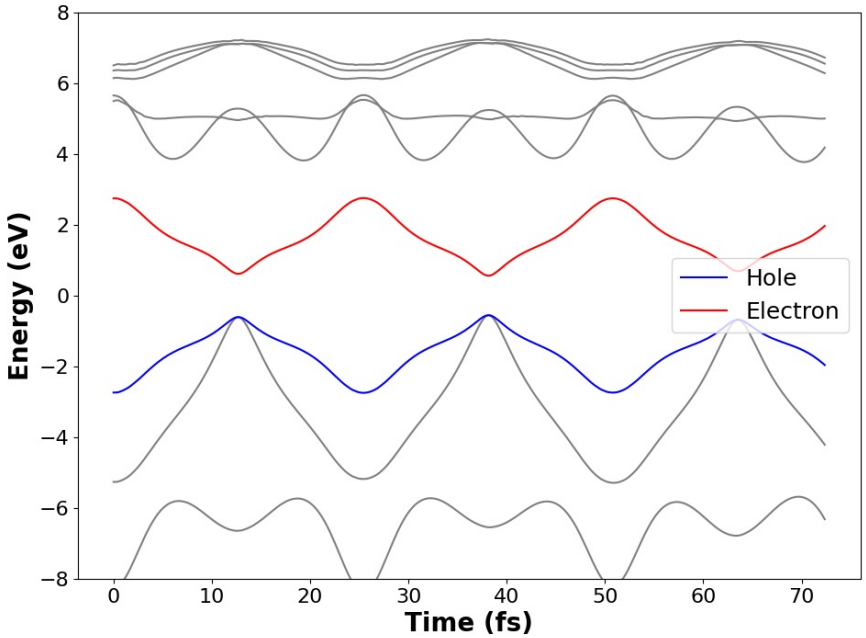


4. Non-adiabatic Quantum Molecular Dynamics (NAQMD)

Trajectory Visualization



wavefunction isosurfaces
（ excited electron (pink), hole (teal) ）
overlayed on the water molecule.



Recombination Rate (s^{-1}) : 1.644E+09