

QXMD Hands-on Session

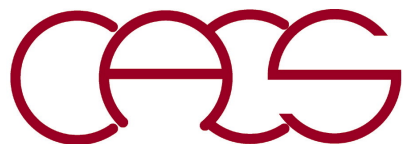
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Himani Mishra, Liqui Yang, Jingxin Zhang**

Collaboratory for Advanced Computing & Simulations

University of Southern California

CyberMAGICS Workshop

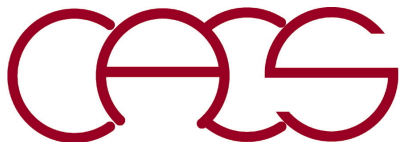
June 30, 2023



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

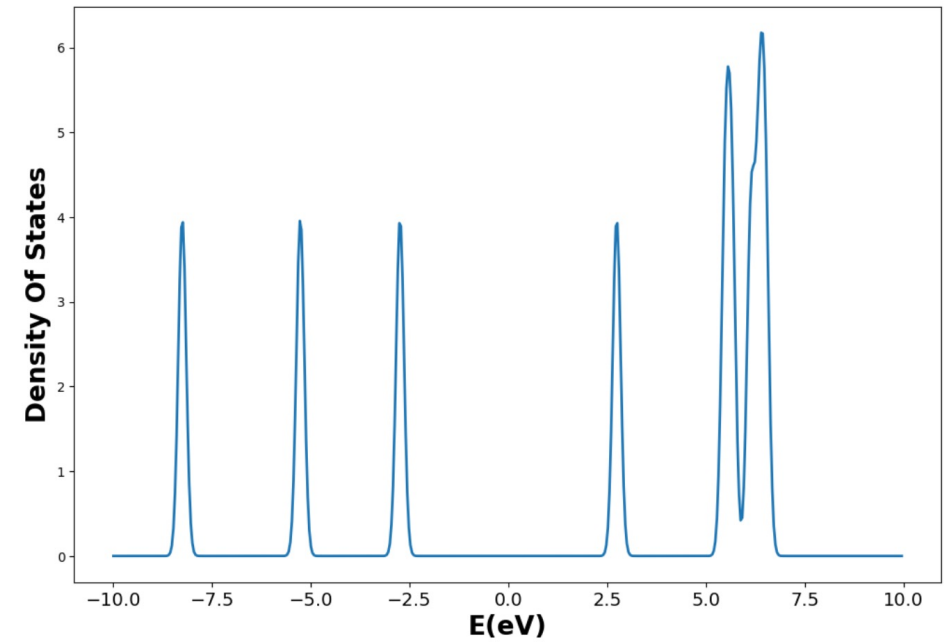
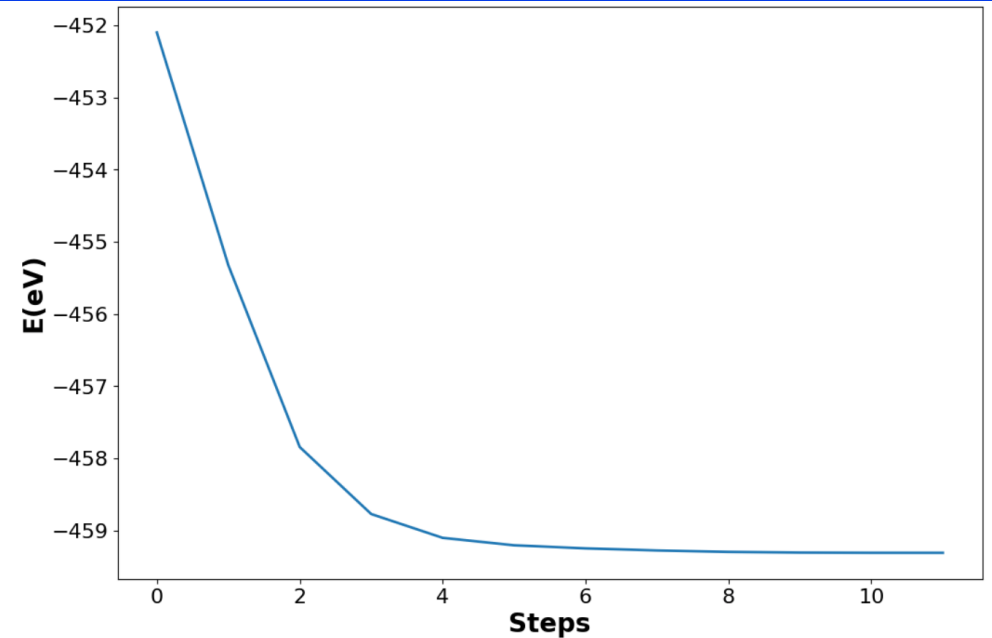
0: Conjugate gradient

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

liscale: .false.

iscnum: 25

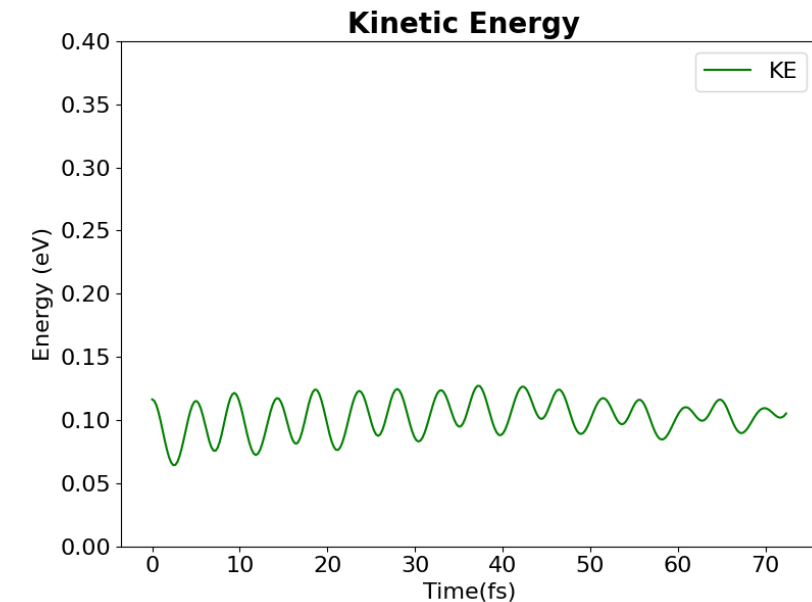
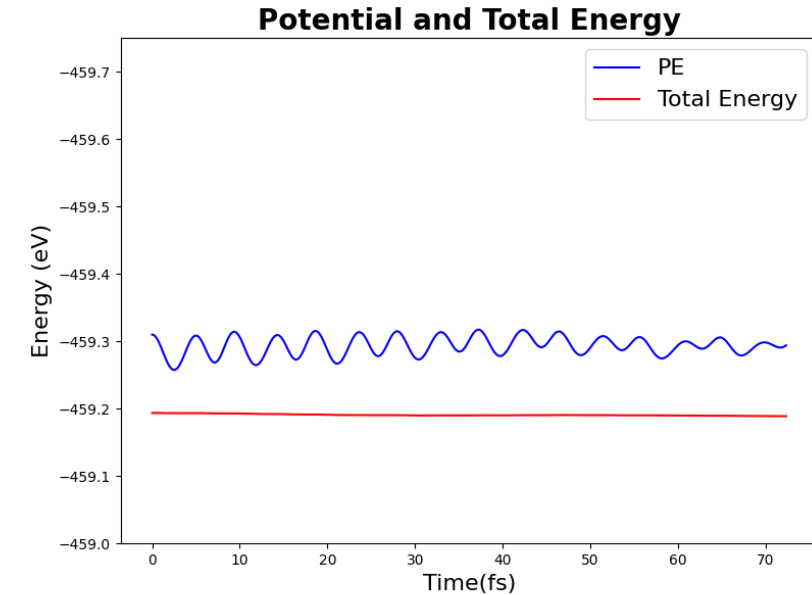
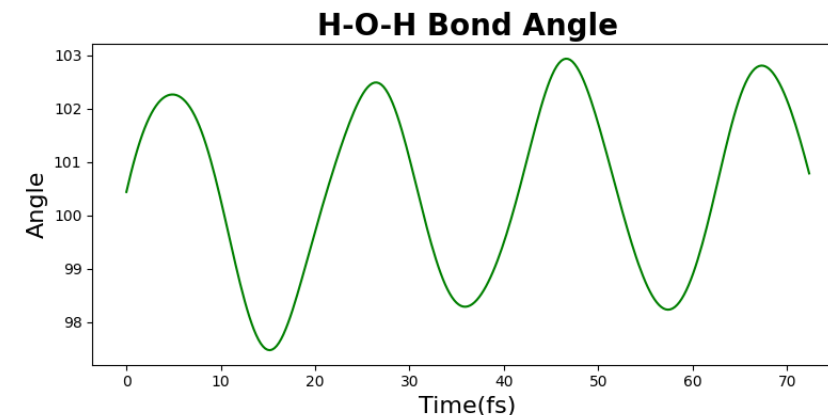
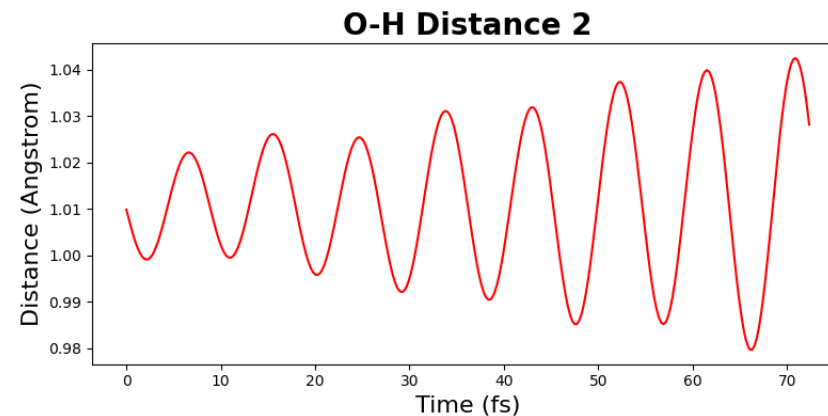
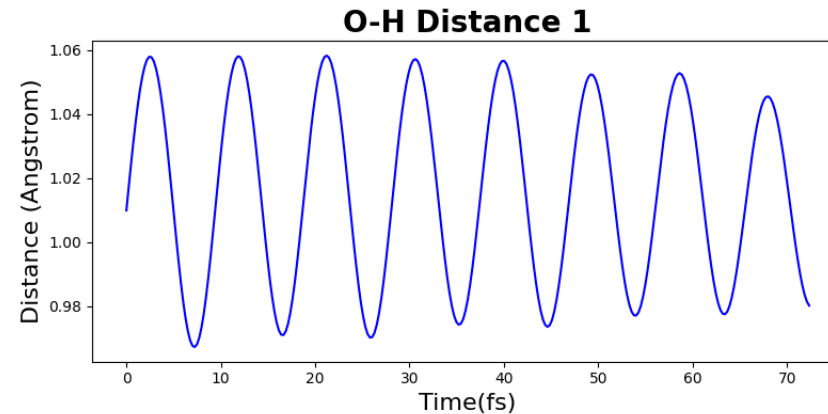
iscstp: 20

ioskip: 1

locoor: .true.

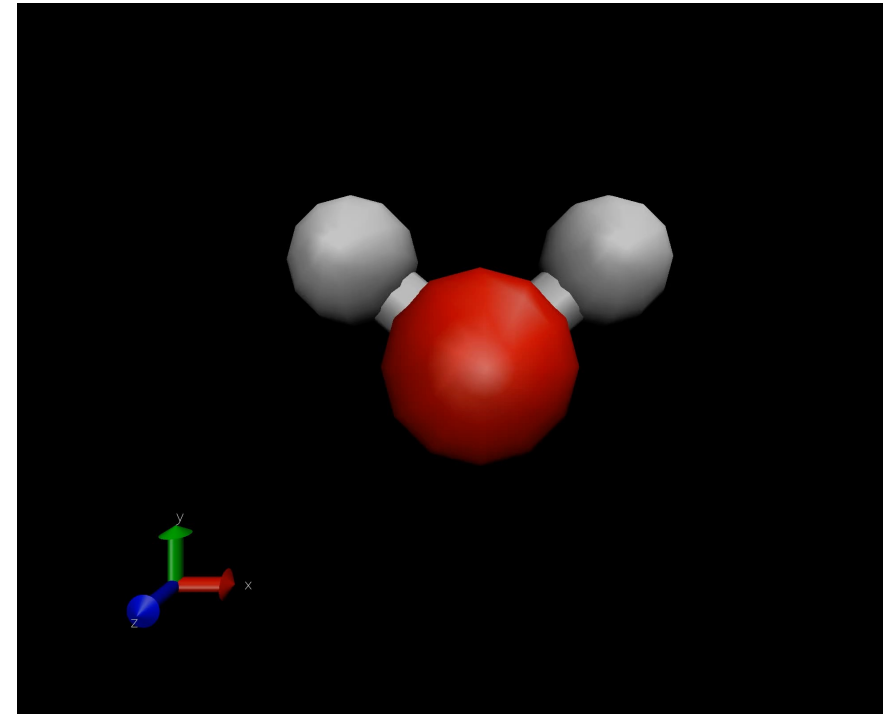
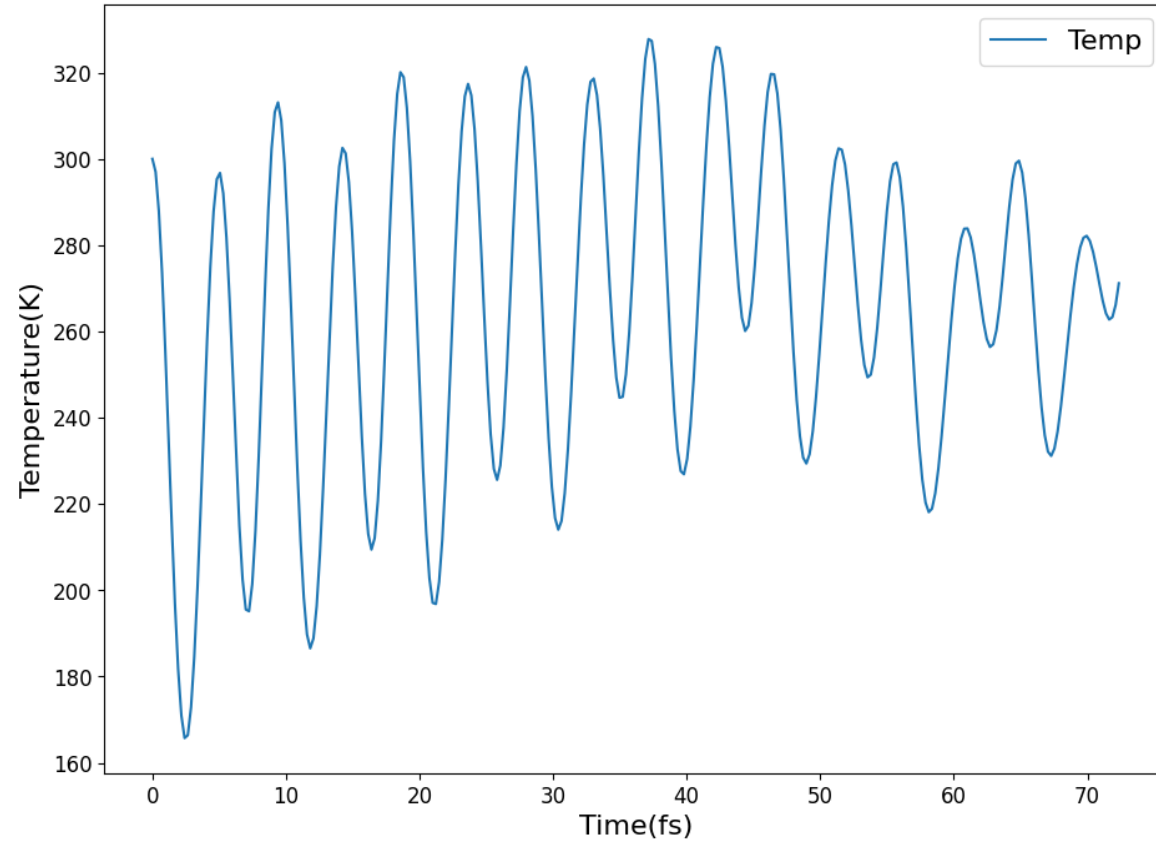
lovelo: .true.

loforc: .true.



3. Adiabatic Quantum Molecular Dynamics (QMD)

Trajectory Visualization



4. Non-adiabatic Quantum Molecular Dynamics (NAQMD)

*molecular dynamics

*TDDFT-MD

ifmd: 2

dtmd: 10.0d0

nstop: 300

treq: 0.1d0

liscale: .false.

iscnum: 25

iscstp: 20

ioskip: 1

locoor: .true.

lovelo: .true.

loforc: .true.

ltddft: .true.

ltddft_fssh : .true.

lfssh_gsscf: .true.

aslh_fssh: 0.8d0

bslh_fssh: 0.13d0

dtddft: 0.04d0

ltddft_start: .false.

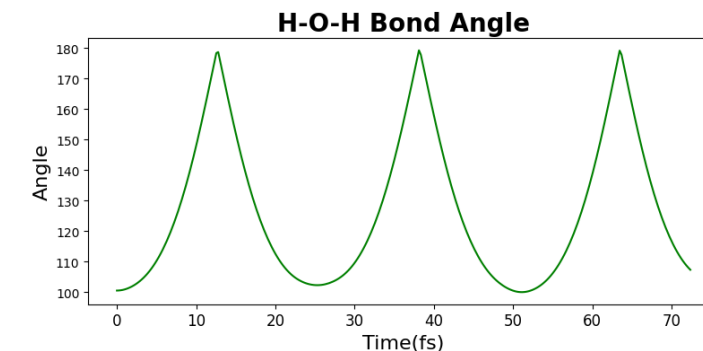
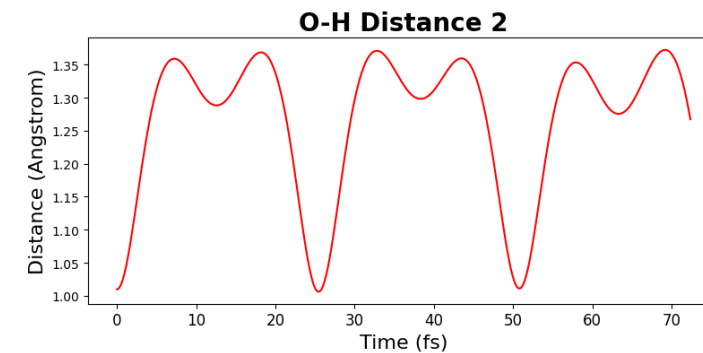
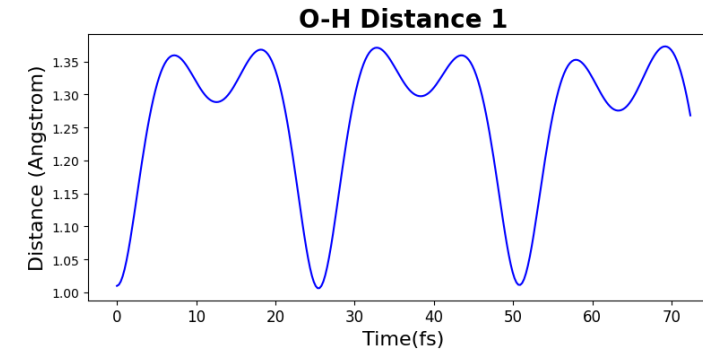
lfssh_random: .true.

rseed_fssh:1119041003.0000000

nocc_change: 2

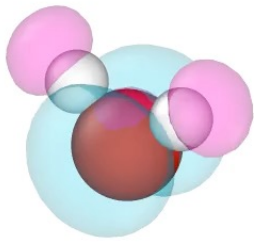
numband: 4

occ_new: 1.0 0.0

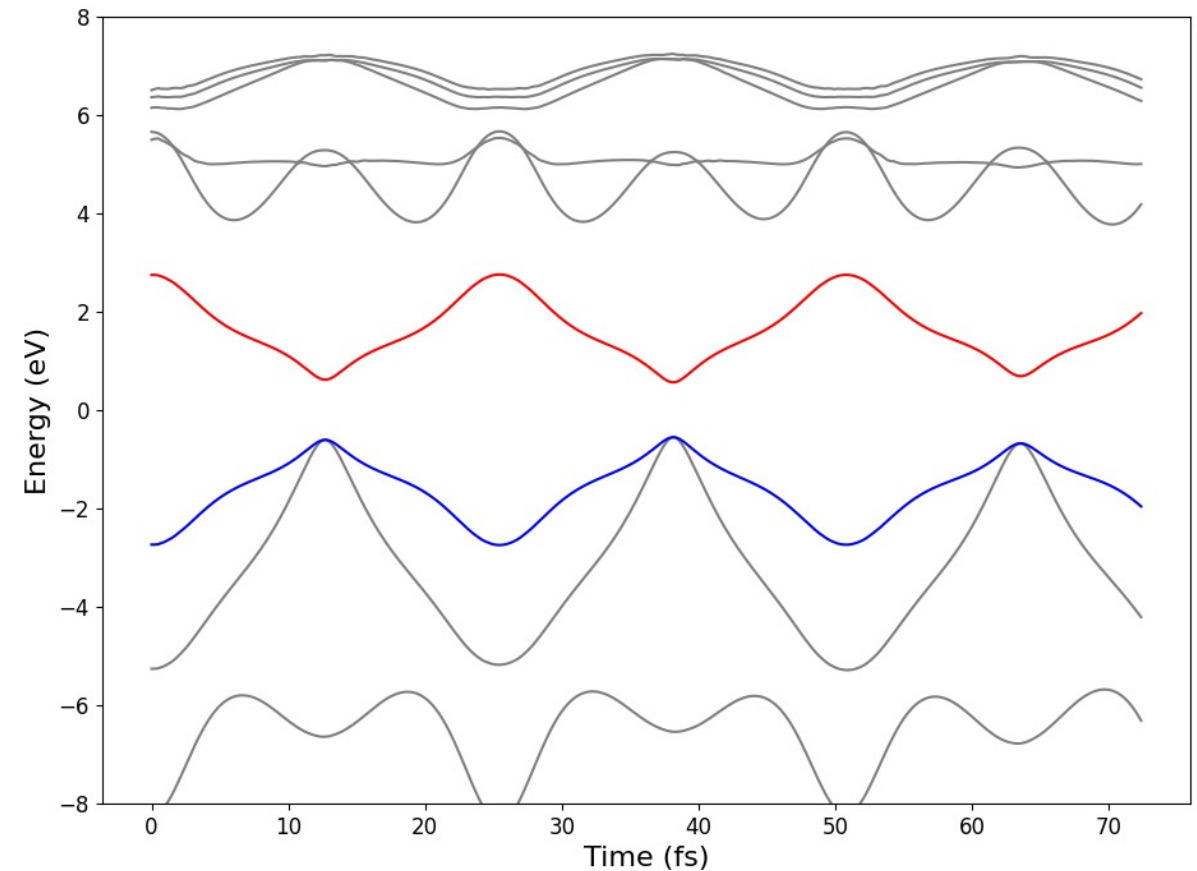


4. Non-adiabatic Quantum Molecular Dynamics (NAQMD)

Trajectory Visualization



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



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