Please email glenn.r.pastel.civ@army.mil for requests and questions regarding the BOMD simulations.

Contents of 'bomd_AlH2O6__4_OTf__12_H2O__40_800K_trajectories.tar.gz' tarball:

.

./0readme.md

./al__4_otf__12_h2o__40_run__5-pos-1.dcd

./al__4_otf__12_h2o__40_run__5.restart

./al__4_otf__12_h2o__40_run__6-pos-1.dcd

./al__4_otf__12_h2o__40_run__6.restart

./al__4_otf__12_h2o__40_run__7-pos-1.dcd

./al__4_otf__12_h2o__40_run__7.restart

./al__4_otf__12_h2o__40_run__8-pos-1.dcd

./al__4_otf__12_h2o__40_run__8.restart

./batch_convert.sh

./convert_to_xyz.py

./files_to_continue_trajectories

./files_to_continue_trajectories/al__4_otf__12_h2o__40_run__5-1.restart

./files_to_continue_trajectories/al__4_otf__12_h2o__40_run__5-RESTART.wfn

./files_to_continue_trajectories/al__4_otf__12_h2o__40_run__6-1.restart

./files_to_continue_trajectories/al__4_otf__12_h2o__40_run__6-RESTART.wfn

./files_to_continue_trajectories/al__4_otf__12_h2o__40_run__7-1.restart

./files_to_continue_trajectories/al__4_otf__12_h2o__40_run__7-RESTART.wfn

./files_to_continue_trajectories/al__4_otf__12_h2o__40_run__8-1.restart

./files_to_continue_trajectories/al__4_otf__12_h2o__40_run__8-RESTART.wfn

dcd and wfn files are binary. An example of the restart file is given at the end, only the header contains any potentially identifying info (date and time of simulation, name of machine run on, and scratch/temporary directory the simulation was run in). I replaced my HPC username with 'scrubbed' in each file. The name of the computer Narwhal is unclassified and date and time of simulation is simply a timestamp.

0readme.md

README

Filename explanation:

Composition is 4 x [Al(H2O)6] + 12 x OTf + 40 free waters. Reflects how they were built from fragments using Packmol initially. [Al(H2O)6] is just truncated to Al.

Main directory:

- restart: provides XYZ and lattice parameters for conversion
- dcd: binary format of trajectory
- sh: convert all files using the python script
- py: we used ASE v 3.22.0 to convert dcd files to xyz

Recommend using TRAVIS analyzer (by Martin Brehm) to wrap with molecule completion across boundaries, the python script above writes lattice parameters as the comment in the xyz file. TRAVIS reads the cell parameters from comment card of xyz file.

Note that the O and H atoms of water are called O and H to be read into ASE.

files_to_continue_trajectories directory:

- -1.restart: final snapshot from CP2K, use to continue simulations
- -RESTART.wfn: wave function from final snapshot

Note that the O and H atoms of water are called HW and OW here.

batch_conversion.sh:

```
#!/bin/bash


function conv2xyz () {
  python3 convert_to_xyz.py $1 $2 $3 &
}


for i in 5 6 7 8; do conv2xyz al__4_otf__12_h2o__40_run__$i\.restart
al__4_otf__12_h2o__40_run__$i\-pos-1.dcd al__4_otf__12_h2o__40_run__$i; done
```

convert_to_xyz.py:

```
#!/usr/bin/env python3

'''
 python3 convert_to_xyz.py foo.restart foo-pos-1.dcd foo

 Converts CP2K restart and DCD (not aligned) to XMOL format
'''

import sys
import ase

from ase.io import read, write
from ase.io.cp2k import iread_cp2k_dcd, read_cp2k_restart
from ase.calculators.cp2k import CP2K

rst = sys.argv[1]
dcd = sys.argv[2]
out = sys.argv[3]

ref = read(rst, format='cp2k-restart')
with open(dcd, 'rb') as f:
   idcd = iread_cp2k_dcd(f, indices=slice(0,None), ref_atoms=ref, aligned=False) # change to True is DCD_ALIGNED_CELL is used
   for image in idcd:
      image.set_cell(ref.cell)
      image.set_pbc([True, True, True])
      image.wrap()
```

```
        write('%s.xyz' % (out), image, format='xyz', comment="%s" % ('
'.join(map(str,image.get_cell_lengths_and_angles()))), append=True)
```

```
# Version information for this restart file
 # current date 2021-11-28 16:26:15.424
 # current working dir /p/work1/scrubbed/1687674.narwhal-pbs
 # Program compiled at                Tue Jun 22 00:11:24 GMT 2021
 # Program compiled on                           narwhal04
 # Program compiled for                   CRAY-XC40-Narwhal
 # Source code revision number                   git:310b7ab
 &GLOBAL
  PREFERRED_FFT_LIBRARY  FFTW3
  FFTW_PLAN_TYPE  MEASURE
  EXTENDED_FFT_LENGTHS  T
  PRINT_LEVEL  LO
  PROJECT_NAME al__4_otf__12_h2o__40_run__5
  RUN_TYPE  MD
  WALLTIME 603000
 &END GLOBAL
 &MOTION
  &MD
   ENSEMBLE  NVT
   STEPS  2000
   MAX_STEPS  500000
   TIMESTEP     4.9999999999999989E-01
   STEP_START_VAL  64000
   TIME_START_VAL     3.1999999999977634E+04
   TEMPERATURE     8.0015000000000009E+02
   COMVEL_TOL     9.9999999999999998E-17
   &THERMOSTAT
    TYPE  CSVR
```

```
    REGION  GLOBAL
    &CSVR
      TIMECON     1.1000000000000000E+01
    &END CSVR
  &END THERMOSTAT
  &PRINT
    &ENERGY  SILENT
      &EACH
        MD  4
      &END EACH
    &END ENERGY
  &END PRINT
&END MD
&PRINT
  &TRAJECTORY  SILENT
    FORMAT  DCD
    &EACH
      MD  4
    &END EACH
  &END TRAJECTORY
  &CELL  SILENT
    &EACH
      MD  4
    &END EACH
  &END CELL
  &VELOCITIES  SILENT
    FORMAT  DCD
    &EACH
```

```
      MD  4
     &END EACH
    &END VELOCITIES
    &FORCES  SILENT
     FORMAT  DCD
     &EACH
      MD  4
     &END EACH
    &END FORCES
    &STRESS  SILENT
     &EACH
      MD  4
     &END EACH
    &END STRESS
   &END PRINT
&END MOTION
&FORCE_EVAL
  METHOD  QS
  STRESS_TENSOR  ANALYTICAL
  &DFT
    BASIS_SET_FILE_NAME data/BASIS_MOLOPT
    POTENTIAL_FILE_NAME data/POTENTIAL
    WFN_RESTART_FILE_NAME al__4_otf__12_h2o__40_run__5-RESTART.wfn
    UKS  F
    MULTIPLICITY  1
    CHARGE  0
    &SCF
     MAX_SCF  60
```

```
 EPS_SCF     9.9999999999999995E-07
 SCF_GUESS  RESTART
 &OT  T
  MINIMIZER  DIIS
 &END OT
 &OUTER_SCF  T
  EPS_SCF     9.9999999999999995E-07
  MAX_SCF  10
 &END OUTER_SCF
&END SCF
&QS
 EPS_DEFAULT     1.0000000000000000E-13
 METHOD  GPW
&END QS
&MGRID
 NGRIDS  5
 CUTOFF     8.5000000000000000E+02
 REL_CUTOFF     6.0000000000000000E+01
&END MGRID
&XC
 DENSITY_CUTOFF     1.0000000000000000E-13
 GRADIENT_CUTOFF     1.0000000000000000E-13
 TAU_CUTOFF     1.0000000000000000E-13
 &XC_FUNCTIONAL  NO_SHORTCUT
  &PBE  T
   PARAMETRIZATION  REVPBE
  &END PBE
 &END XC_FUNCTIONAL
```

```
      &VDW_POTENTIAL
       POTENTIAL_TYPE  PAIR_POTENTIAL
       &PAIR_POTENTIAL
        TYPE  DFTD3(BJ)
        PARAMETER_FILE_NAME data/dftd3.dat
        REFERENCE_FUNCTIONAL revPBE
       &END PAIR_POTENTIAL
      &END VDW_POTENTIAL
    &END XC
    &POISSON
     POISSON_SOLVER  PERIODIC
     PERIODIC  XYZ
    &END POISSON
  &END DFT
  &SUBSYS
    &CELL
     A    1.5402302000000002E+01    0.0000000000000000E+00    0.0000000000000000E+00
     B    0.0000000000000000E+00    1.5402302000000002E+01    0.0000000000000000E+00
     C    0.0000000000000000E+00    0.0000000000000000E+00    1.5402302000000002E+01
     PERIODIC  XYZ
     MULTIPLE_UNIT_CELL  1 1 1
     SYMMETRY  CUBIC
    &END CELL
    &COORD
O    5.3047742814995598E+00    1.1971217767687361E+00    3.6657729353423640E+00
H    5.1909916769293165E+00    7.2652637145120136E-01    2.8668586612254390E+00
H    4.9320625118432160E+00    4.4902251177452740E-01    4.3073083763048263E+00
… 292 lines like this…
```

```
    &END COORD
    &VELOCITY
        5.6786334699758978E-05    8.9720066437396642E-06    4.4956204300503478E-04
       -8.8514351295429787E-04   -2.3313725759453990E-04   -1.0247202401963652E-03
       -2.5718187714218998E-04    2.2116080665977229E-04    6.2702368224607711E-04
… 292 lines like this…
    &END VELOCITY
    &KIND Al
      BASIS_SET DZVP-MOLOPT-SR-GTH
      POTENTIAL GTH-PBE
      &POTENTIAL
2 1
0.4500000000000000E+00 1 -0.7554761260000000E+01
2
0.4874352900000000E+00 2  0.6959938320000000E+01 -0.1888835840000000E+01
0.2438476590000000E+01
0.5621894900000000E+00 1  0.1865298570000000E+01
      &END POTENTIAL
    &END KIND
    &KIND H
      BASIS_SET DZVP-MOLOPT-SR-GTH
      ELEMENT H
      POTENTIAL GTH-PBE
      &POTENTIAL
1
0.2000000000000000E+00 2 -0.4178900440000000E+01  0.7244633100000000E+00
0
      &END POTENTIAL
```

```
    &END KIND
    &KIND C
      BASIS_SET DZVP-MOLOPT-SR-GTH
      POTENTIAL GTH-PBE
      &POTENTIAL
2 2
0.3384712400000000E+00 2 -0.8803673979999999E+01  0.1339210850000000E+01
2
0.3025757500000000E+00 1  0.9622486650000001E+01
0.2915069400000000E+00 0
      &END POTENTIAL
    &END KIND
    &KIND O
      BASIS_SET DZVP-MOLOPT-SR-GTH
      POTENTIAL GTH-PBE
      &POTENTIAL
2 4
0.2445543000000000E+00 2 -0.1666721480000000E+02  0.2487311320000000E+01
2
0.2209559200000000E+00 1  0.1833745811000000E+02
0.2113324700000000E+00 0
      &END POTENTIAL
    &END KIND
    &KIND O
      BASIS_SET DZVP-MOLOPT-SR-GTH
      ELEMENT O
      POTENTIAL GTH-PBE
      &POTENTIAL
```

2 4

0.2445543000000000E+00 2 -0.1666721480000000E+02 0.2487311320000000E+01

2

0.2209559200000000E+00 1 0.1833745811000000E+02

0.2113324700000000E+00 0

&END POTENTIAL

&END KIND

&KIND F

BASIS_SET DZVP-MOLOPT-SR-GTH

POTENTIAL GTH-PBE

&POTENTIAL

2 5

0.2149295900000000E+00 2 -0.2157302836000000E+02 0.3199776150000000E+01

2

0.1946840200000000E+00 1 0.2374354045000000E+02

0.1861560800000000E+00 0

&END POTENTIAL

&END KIND

&KIND S

BASIS_SET DZVP-MOLOPT-SR-GTH

POTENTIAL GTH-PBE

&POTENTIAL

2 4

0.4200000000000000E+00 1 -0.5986260380000000E+01

2

0.3648203500000000E+00 2 0.1314354448000000E+02 -0.4241830450000000E+01

0.5476179570000000E+01

0.4094804800000000E+00 1 0.3700890570000000E+01

```
    &END POTENTIAL
   &END KIND
   &TOPOLOGY
    NUMBER_OF_ATOMS  292
    CONN_FILE_FORMAT  OFF
    MULTIPLE_UNIT_CELL  1 1 1
   &END TOPOLOGY
  &END SUBSYS
&END FORCE_EVAL
```