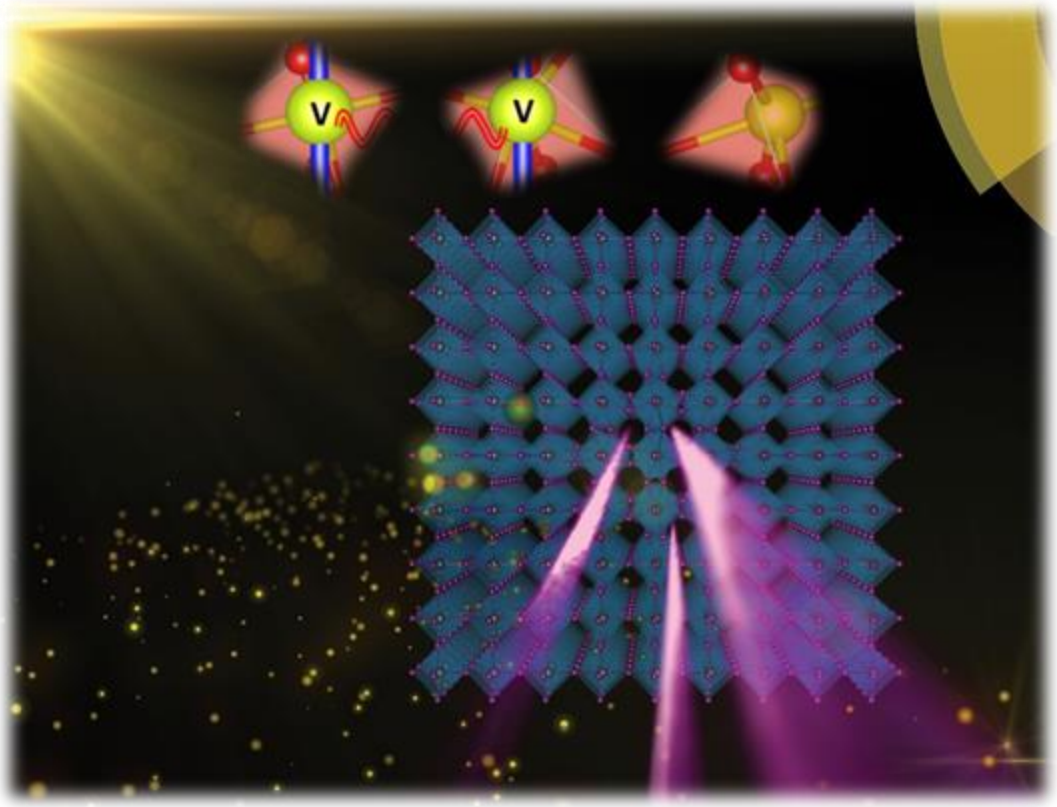
DFT Hands-on H_2O relaxation

https://www.vasp.at/tutorials/latest/molecules/part3/



Byungkyun Kang

bkang@udel.edu

Computational Materials Physics Bootcamp at UD August 2024

Prepare four input files - POTCAR

Download H2O_relaxation files into desktop

Use WinScp to copy H2O_relaxation files into Keldysh (XXX@keldysh.physics.udel.edu)

Go to work directory (XXX/relaxation) using ssh

ssh XXX@keldysh.physics.udel.edu

Check files

relaxation$ ls

```
[bkang@keldysh relaxation]$ :/home/bkang/bootcamp/h2o/relaxation~>ls
INCAR  job.qs  KPOINTS  POSCAR  POSCAR_template  pot
[bkang@keldysh relaxation]$ :/home/bkang/bootcamp/h2o/relaxation~>
```

Create POTCAR

relaxation$ cat ./pot/O/POTCAR ./pot/H/POTCAR > POTCAR

Prepare four input files- POSCAR

```
relaxation~>vi POSCAR_template
```

```
H2O                    ! my name for the system
?                      ! scaling parameter
 ? 0 0                 ! lattice vector a
 0 ? 0                 ! lattice vector b
 0 0 ?                 ! lattice vector c
O H
? ?                    ! number of atoms
cart                   ! positions in cartesian coordinates
      0.00      0.00      0.00
      ?         ?         0.00
      ?         ?         0.00
```

Enter ?

relaxation~>cp POSCAR_template POSCAR

Prepare four input files

INCAR

```
ISMEAR = 0
SIGMA  = 0.1


ENCUT = 520      ! largest ENMAX from POTCAR +30%


IBRION = 1       ! use DIIS algorithm to converge
NSW = 100         ! 10 ionic steps
EDIFFG = -0.02    ! forces smaller 0.02 A/eV
```

KPOINTS

```
Gamma-point
only
 0
Monkhorst Pack
 1 1 1
 0 0 0
```

Run job

Relaxation->./job.qs

job.qs

```
#!/bin/bash
module load vasp/5.4.4
ulimit -s unlimited
mpirun -np 4 vasp_std
```

Check OUTPUT

```
vasp.5.4.4.18Apr17-6-g9f103f2a35 (build Aug 12 2024 15:07:40) complex

executed on             LinuxIFC date 2024.08.12  16:39:49
running on    4 total cores
distrk:  each k-point on    4 cores,    1 groups
distr:  one band on NCORES_PER_BAND=   1 cores,    4 groups


-----------------------------------------------------------------------------
-----------


INCAR:
POTCAR:    PAW_PBE O 08Apr2002
```

```
General timing and accounting informations for this job:
========================================================

                  Total CPU time used (sec):       33.978
                            User time (sec):       31.124
                          System time (sec):        2.854
                         Elapsed time (sec):       34.148

                   Maximum memory used (kb):      195936.
                   Average memory used (kb):           0.

                          Minor page faults:       468912
                          Major page faults:            0
                 Voluntary context switches:          273
```

Check OUTPUT

```
E-fermi :  -6.1471     XC(G=0):  -0.4112     alpha+bet : -0.0753


k-point      1 :       0.0000    0.0000    0.0000
 band No.  band energies     occupation
      1      -22.5226       2.00000
      2       -9.7302       2.00000
      3       -9.3143       2.00000
      4       -6.6568       2.00000
      5       -3.2354       0.00000
      6       -2.1644       0.00000
      7       -0.0168       0.00000
      8        0.6902       0.00000
```

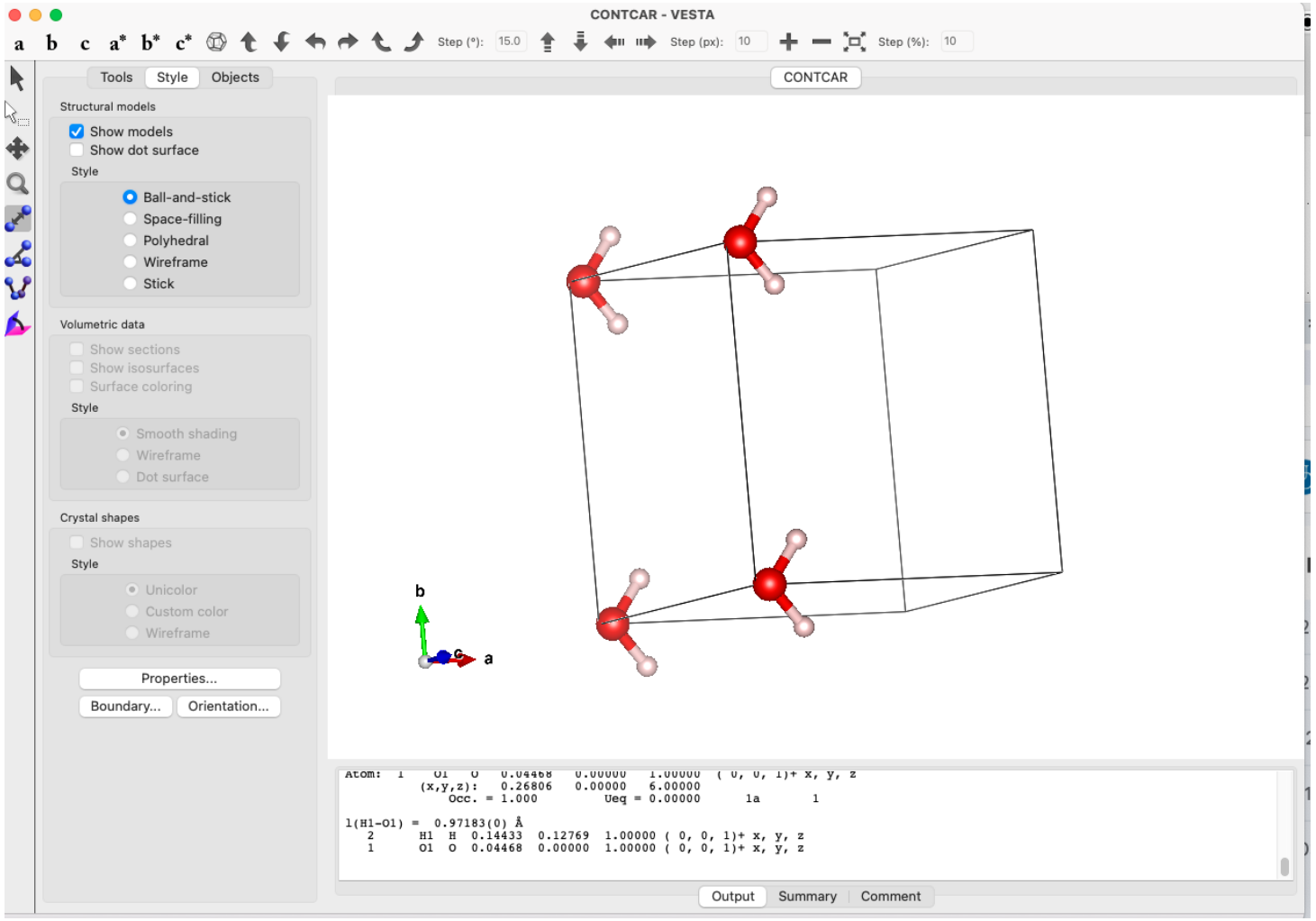
Check OSZICAR

```
[bkang@keldysh test]$ :/home/bkang/bootcamp/h2o/relaxation/test~>grep F OSZICAR
   1 F= -.10358316E+02 E0= -.10358316E+02  d E =-.103583E+02
   2 F= -.13912106E+02 E0= -.13912106E+02  d E =-.355379E+01
   3 F= -.13801588E+02 E0= -.13801588E+02  d E =0.110518E+00
   4 F= -.14186241E+02 E0= -.14186241E+02  d E =-.384653E+00
   5 F= -.14218808E+02 E0= -.14218808E+02  d E =-.325669E-01
   6 F= -.14219515E+02 E0= -.14219515E+02  d E =-.707956E-03
   7 F= -.14220719E+02 E0= -.14220719E+02  d E =-.120337E-02
[bkang@keldysh test]$ :/home/bkang/bootcamp/h2o/relaxation/test~>
```

Check CONTCAR

winscp: transfer CONTCAR to desktop

vesta: what is bond length and angle?



Thank you