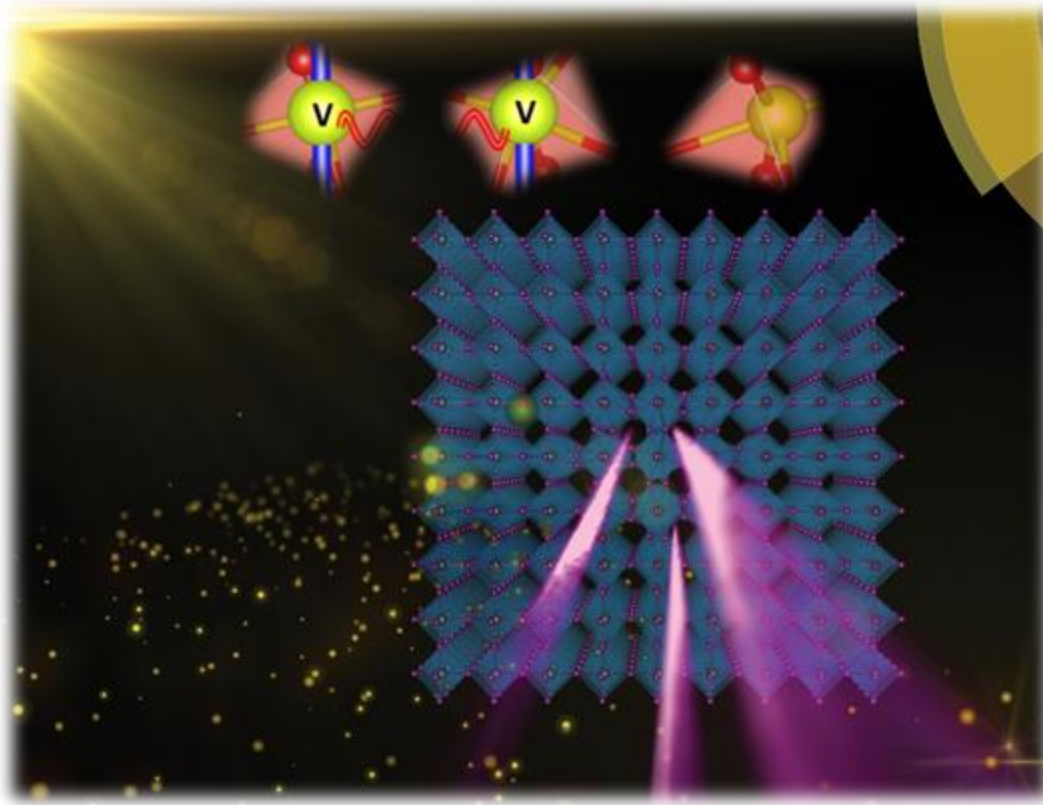


DFT Hands-on H₂O vibration

<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

Download H2O_vibration files into desktop

Use WinScp to copy H2O_vibration files into Keldysh (XXX@keldysh.physics.udel.edu)

Go to work directory (XXX/vibration) using ssh

```
ssh XXX@keldysh.physics.udel.edu
```

Check files

```
vibration$ ls
```

```
[bkang@keldysh vibration]$ :/home/bkang/bootcamp/h2o/vibration~>ls  
IBRION6  IBRION8  
[bkang@keldysh vibration]$ :/home/bkang/bootcamp/h2o/vibration~>
```

Run jobs

IBRION6/
./job.qs

second derivatives, Hessian matrix, and phonon frequencies
(finite differences)

IBRION8/
./job.qs

second derivatives, Hessian matrix, and phonon frequencies
(perturbation theory)

Find vibrational eigenvectors and eigenvalues in OUTCAR

IBRION6

```
1 f = 115.415114 THz 725.174549 2PiTHz 3849.833691 cm-1 477.318715 meV
      X      Y      Z      dx      dy      dz
0.000000 0.000000 0.000000 -0.000000 0.269005 -0.000000
0.595641 5.582786 0.000000 0.417500 -0.538063 -0.000000
0.595641 0.767374 0.000000 -0.417500 -0.538063 -0.000000
```

```
2 f = 112.164387 THz 704.749626 2PiTHz 3741.401101 cm-1 463.874783 meV
      X      Y      Z      dx      dy      dz
0.000000 0.000000 0.000000 -0.192043 -0.000000 0.000000
0.595641 5.582786 0.000000 0.384108 -0.577945 0.000000
0.595641 0.767374 0.000000 0.384108 0.577945 0.000000
```

```
3 f = 47.630429 THz 299.270815 2PiTHz 1588.780062 cm-1 196.983693 meV
      X      Y      Z      dx      dy      dz
0.000000 0.000000 0.000000 -0.272334 0.000000 -0.000000
0.595641 5.582786 0.000000 0.544920 0.407406 -0.000000
0.595641 0.767374 0.000000 0.544920 -0.407406 0.000000
```

```
4 f = 0.107570 THz 0.675881 2PiTHz 3.588143 cm-1 0.444873 meV
      X      Y      Z      dx      dy      dz
0.000000 0.000000 0.000000 0.000000 0.000000 0.931499
0.595641 5.582786 0.000000 0.000000 0.000000 0.257206
0.595641 0.767374 0.000000 0.000000 0.000000 0.257206
```

```
5 f = 0.057740 THz 0.362791 2PiTHz 1.925998 cm-1 0.238793 meV
      X      Y      Z      dx      dy      dz
0.000000 0.000000 0.000000 -0.000000 -0.940018 0.000000
0.595641 5.582786 0.000000 -0.007864 -0.241084 0.000000
0.595641 0.767374 0.000000 0.007864 -0.241084 0.000000
```

```
6 f/i= 0.005775 THz 0.036283 2PiTHz 0.192623 cm-1 0.023882 meV
      X      Y      Z      dx      dy      dz
0.000000 0.000000 0.000000 0.942843 -0.000000 -0.000000
0.595641 5.582786 0.000000 0.235634 -0.000043 -0.000000
0.595641 0.767374 0.000000 0.235634 0.000043 -0.000000
```

```
7 f/i= 3.314068 THz 20.822902 2PiTHz 110.545401 cm-1 13.705888 meV
      X      Y      Z      dx      dy      dz
0.000000 0.000000 0.000000 -0.000000 -0.000000 0.363744
0.595641 5.582786 0.000000 -0.000000 -0.000000 -0.658669
0.595641 0.767374 0.000000 -0.000000 -0.000000 -0.658669
```

```
8 f/i= 3.726135 THz 23.411997 2PiTHz 124.290484 cm-1 15.410062 meV
      X      Y      Z      dx      dy      dz
```

IBRION8

```
1 f = 115.380705 THz 724.958352 2PiTHz 3848.685938 cm-1 477.176412 meV
      X      Y      Z      dx      dy      dz
0.000000 0.000000 0.000000 0.000000 0.268958 -0.000000
0.595641 5.582786 0.000000 0.417523 -0.538057 -0.000000
0.595641 0.767374 0.000000 -0.417523 -0.538057 -0.000000
```

```
2 f = 112.132348 THz 704.548323 2PiTHz 3740.332417 cm-1 463.742283 meV
      X      Y      Z      dx      dy      dz
0.000000 0.000000 0.000000 -0.192021 0.000000 0.000000
0.595641 5.582786 0.000000 0.384131 -0.577934 0.000000
0.595641 0.767374 0.000000 0.384131 0.577934 0.000000
```

```
3 f = 47.687472 THz 299.629223 2PiTHz 1590.682796 cm-1 197.219602 meV
      X      Y      Z      dx      dy      dz
0.000000 0.000000 0.000000 -0.272137 0.000000 -0.000000
0.595641 5.582786 0.000000 0.544957 0.407422 -0.000000
0.595641 0.767374 0.000000 0.544957 -0.407422 0.000000
```

```
4 f = 0.300547 THz 1.888395 2PiTHz 10.025183 cm-1 1.242965 meV
      X      Y      Z      dx      dy      dz
0.000000 0.000000 0.000000 0.000000 0.000000 0.912741
0.595641 5.582786 0.000000 0.000000 0.000000 0.288880
0.595641 0.767374 0.000000 -0.000000 0.000000 0.288880
```

```
5 f = 0.172524 THz 1.084000 2PiTHz 5.754778 cm-1 0.713502 meV
      X      Y      Z      dx      dy      dz
0.000000 0.000000 0.000000 -0.000000 -0.932412 0.000000
0.595641 5.582786 0.000000 -0.027139 -0.254102 0.000000
0.595641 0.767374 0.000000 0.027139 -0.254102 0.000000
```

```
6 f/i= 0.016049 THz 0.100836 2PiTHz 0.535323 cm-1 0.066372 meV
      X      Y      Z      dx      dy      dz
0.000000 0.000000 0.000000 0.942905 -0.000000 -0.000000
0.595641 5.582786 0.000000 0.235511 -0.000107 -0.000000
0.595641 0.767374 0.000000 0.235511 0.000107 -0.000000
```

```
7 f/i= 3.630972 THz 22.814070 2PiTHz 121.116184 cm-1 15.016498 meV
      X      Y      Z      dx      dy      dz
0.000000 0.000000 0.000000 -0.000000 -0.241391 -0.000000
0.595641 5.582786 0.000000 0.570033 0.382004 0.000000
0.595641 0.767374 0.000000 -0.570033 0.382004 0.000000
```

```
8 f/i= 3.701645 THz 23.258122 2PiTHz 123.473587 cm-1 15.308779 meV
      X      Y      Z      dx      dy      dz
```

Thank you