Phonon:

INCAR

SYSTEM = Si\_bulk

ISTART = 0 # From-scratch; job : 0-new 1-cont 2-samecut

NWRITE = 3 Verbosity

! electronic relaxation

ENCUT = 300.0 # cut-off energy

PREC = Accurate # precision : accurate/normal/low

ISPIN = 1 # 1 - off, 2 - on (non spin-polarized calculation)

ICHARG = 2 # > 10 for non-SC calculation

IALGO = 38 # DAVidson, then RMM-DIIS

EDIFF = 1.0E-8 # default

ISMEAR = 0 # gaussian

SIGMA = 0.05

! PAW's

LREAL = .FALSE. # default - Automatic choice of how projection is done

ADDGRID = .TRUE.

! phonons

IBRION = 5

POTIM = 0.01

! parallelisation

LPLANE = .FALSE.

KPAR=8

! output

LWAVE = .FALSE. # WAVECAR file

LCHARG = .FALSE. # CHCAR file

LELF = .FALSE.

LVTOT = .FALSE.

KPOINTS:

Automatic mesh

0 ! number of k-points = 0 ->automatic generation scheme

M ! generate a Gamma centered grid

4 4 4

0.5 0.5 0.5

Script to run Phonon

#!/bin/bash

#SBATCH --time=10:00:00

#SBATCH -N 4

#SBATCH --account=snic2019-1-25

#SBATCH -J Phonon

#SBATCH --exclusive

#SBATCH --ntasks-per-node=32

module load VASP/5.4.4.16052018-nsc1-intel-2018b-eb

mpprun vasp\_std

RAMAN

Create a folder named Raman:

Copy vasp\_raman.py to the folder

Copy OUTCAR and rename to OUTCAR.phon and paste to Raman directory from Phonon Folder.

Same with CONTCAR and rename to POSCAR.phon

Copy EIGENVAL and paste to Raman folder

INCAR

SYSTEM = NAPTHA04

ISTART = 0 # From-scratch; job : 0-new 1-cont 2-samecut

NWRITE = 3 Verbosity

! electronic relaxation

ENCUT = 400.0 # cut-off energy

PREC = Normal # precision : accurate/normal/low

ISPIN = 1 # 1 - off, 2 - on (non spin-polarized calculation)

ICHARG = 2 # > 10 for non-SC calculation

ALGO = Fast # DAVidson, then RMM-DIIS

EDIFF = 1.0E-8 # default

ISMEAR = 0 # gaussian

SIGMA = 0.02

! PAW's

LREAL = .FALSE. # default - Automatic choice of how projection is done

ADDGRID = .TRUE.

!LCALCEPS=.TRUE.

LEPSILON= .TRUE.

! ionic relaxation

!EDIFFG = -1E-4

!ISYM = 0

!IBRION = 1

!NSW = 1000

! ISIF = 2

! parallelisation

LPLANE = .TRUE.

NSIM=4

!NPAR = 2 # number of cores

! output

LWAVE = .FALSE. # WAVECAR file

LCHARG = .FALSE. # CHCAR file

LELF = .FALSE.

LVTOT = .FALSE.

KPOINTS

Automatic mesh

0 ! number of k-points = 0 ->automatic generation scheme

M ! generate a Gamma centered grid

4 4 4

0.5 0.5 0.5

Do the following in the terminal:

Load Python 2.7.14-anaconda

export VASP\_RAMAN\_RUN="mpprun /software/sse/manual/vasp/5.4.4.16052018/nsc1/vasp\_std"

export VASP\_RAMAN\_PARAMS="01\_24\_2\_0.01"

Script to run RAMAN

#!/bin/bash

#SBATCH --time=05:00:00

#SBATCH -N 4

#SBATCH --account=snic2019-1-25

#SBATCH -J Raman

#SBATCH --exclusive

#SBATCH --ntasks-per-node=32

ulimit -s unlimited

export VASP\_RAMAN\_RUN="mpprun /software/sse/manual/vasp/5.4.4.16052018/nsc1/vasp\_std"

export VASP\_RAMAN\_PARAMS="01\_24\_2\_0.01"

module load Python/2.7.14-anaconda-5.0.1-nsc1

python vasp\_raman.py > vasp\_raman.out

For graph

Broaden.py

Command: python broaden.py vasp\_ramn.dat