STEPS OF ESTIMATING TEMPERATURE DEPENDENT PROPERTIES THROUGH QUASI HARMONIC APPROXIMATION

Step 1

conda activate phonon
relax input structure under vasp_input/GO/
cp vasp_input/GO/CONTCAR POSCAR_unitcell

Step 2

python preprocess.py

Creates bi-axial deformation structures.
Deformation magnitude and direction can be controlled in preprocess.py

Step 3

sh exec_vasp_run_for.sh

Create deformed_structures/static_run/ and run respective static calculations.

Step 3

sh exec_vasp_run_for_DFPT.sh

Create DFPT supercell and run DFPT calculations in VASP for vibration energy.

Step 4

sh post_process_DFPT.sh

Collect force constants from vasprun.xml
Creates thermal_properties.yaml file

Step 5

python post_process.py

Create e-v.dat file in QHA_phonpy_process/e-v.dat

Step 6

python QHA_phonopy_process.py

Creates thermal output files under QHA_phonopy_results/

Step 7

python QHA_manual_process.py

Creates lattice parameter and elastic constants changes with respect to temperature.