Phonopy light intro

Finite difference

`phonopy -d --dim="2 2 3"`

Supercell dimensions
(= cubic for homogenous forces)

Supercell displacements

`phonopy_disp.yaml  POSCAR  POSCAR-001  POSCAR-002  POSCAR-003  SPOSCAR`

Script

KPOINTS
(conserve sampling)

VASP Calculations

INCAR

```
  PREC = Accurate
IBRION = -1
 ENCUT = 500
 EDIFF = 1.0e-08
ISMEAR = 0; SIGMA = 0.01
 IALGO = 38
 LREAL = .FALSE.
 LWAVE = .FALSE.
LCHARG = .FALSE.
```

FORCE_SETS

(with `phonopy_disp.yaml` and `vasprun.xml`)

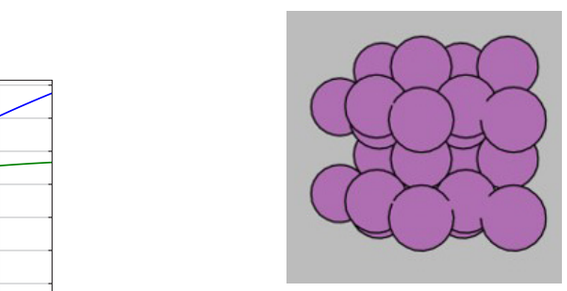
Force constants

Dynamical matrix

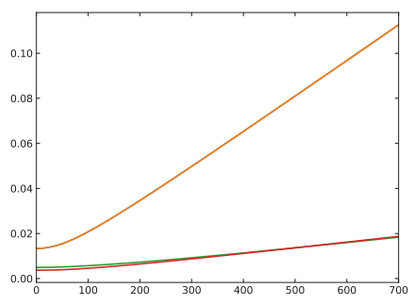
Phonon frequencies and many others...

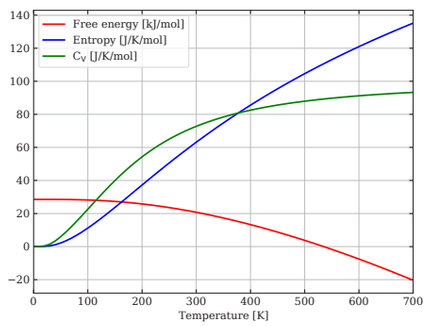
Visualise

with ASCII-phonon

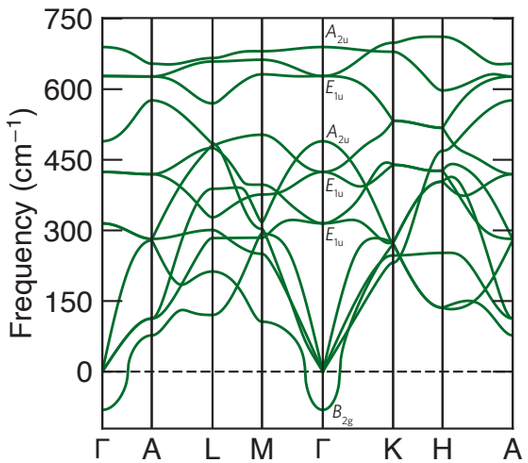


Thermal properties





with SUMO



Band structures

DoS

Symmetry and irreducible representation