1. Structure
   1. Lattice constant: a = 3.267 Å, Δ=1.665 Å
   2. Energy convergence threshold is 1.0d-7 Ryd and force convergence threshold is 1.0d-5 Ryd/Bohr. C length is 26.4 Å, then vacuum layer distance is ~ 23 Å.
   3. The calculation is done on ‘Intel Xeon 6148G’ with one node, 40 cores. The computational time is 54.12s (wall time).
   4. Input file is given under ‘inputs/1.structure/relax.in’
2. Electronic

2.1 Threshold for convergence in the scf calculation is 1.0d-10 Ryd. The kmesh is 6\*6\*1 without grid shifting.

* 1. The convergence evidence can be seen from the Fig. 1 below.

Chart, line chart

Description automatically generatedChart

Description automatically generated with low confidence

Fig.1 Electronic band structure obtained with different kmesh.

* 1. Computational time (all done with 40 cores)

scf: 16.32s with 40 cores

bands.1 52.02s

bands.2 1m39.38s

band.1 56.02s

band.2 49.44s

* 1. Input files are located at ‘data/2.electronic’

1. Harmonic
   1. Converged harmonic force constant is located at ‘data/3.harmonic/espresso.fc’
   2. Dielectric constant

4.7176639 0.0000000 0.0000000

0.0000000 4.7176639 0.0000000

0.0000000 0.0000000 1.2678282

Born effective charge

Mo

-1.8704828 0.0000000 0.0000000

0.0000000 -1.8704828 0.0000000

0.0000000 0.0000000 -0.1370881

Se1

0.9352414 0.0000000 0.0000000

0.0000000 0.9352414 0.0000000

0.0000000 0.0000000 0.0685441

Se2

0.9352414 0.0000000 0.0000000

0.0000000 0.9352414 0.0000000

0.0000000 0.0000000 0.0685441

* 1. Method of long-range Coulomb corrections: DFPT
  2. Thresholds: 1.0d-22

integration mesh: 8\*8\*1

* 1. Convergence evidence

A picture containing chart

Description automatically generatedA picture containing diagram

Description automatically generated

Fig.2 Phonon dispersion relation obtained with different kmesh.

* 1. Computational time: 7h56m with 2\*24 cores
  2. All input files are located at ‘data/3.harmonic’

1. Anharmonic thermal transport
   1. Lattice thermal conductivity v.s. temperature data is stored at ‘data/4.anharmonic/kappa\_vs\_T.csv’
   2. Accumulated lattice thermal conductivity w.r.t mfp is at ‘data/4.anharmonic/ mfp\_kappa.csv’
   3. Accumulated lattice thermal conductivity w.r.t mfp is at ‘data/4.anharmonic/ omega\_kappa.csv’
   4. Scattering rate data is at ‘data/4.anharmonic/sr.csv’
   5. Delta function is represented with adaptive smearing; the integration grid is 120\*120\*1; Symmetry is employed.
   6. Cutoff: 0.677 nm (6th nearest neighbour)
   7. Supercell size: 5\*5\*1
   8. Integration mesh: gamma only
   9. The convergence evidence for lattice thermal conductivity with respect to kmesh can be seen from the Fig. 3 below.

Chart, line chart

Description automatically generated

Fig. 3 Lattice thermal conductivity as function kmesh

* 1. Low temperature w/ isotope (11 data points) takes 15m22s with 40 cores

High temperature w/ isotope (7 data points) takes 12m08s with 40 cores

Low temperature w/o isotope (11 data points) takes 14m53s with 40 cores

High temperature w/o isotope (7 data points) takes 13m51s with 40 cores

* 1. All the input files are stored in ‘data/4.anharmonic/inputs’ folder.