1. Structure&electronic
   1. Lattice constant: a = 7.015 Å
   2. Energy convergence threshold is 1.0d-7 Ryd and force convergence threshold is 1.0d-5 Ryd/Bohr.
   3. Integration mesh is 6\*6\*6 without shifting.
   4. No smearing
   5. Fermi energy 0.8030 eV
   6. The calculation is done on ‘Intel Xeon 6148G’ with one node, 40 cores. The computational time is 19.26s (wall time).
   7. Input file is given under ‘inputs/1.structure&electronic/relax.in’
   8. Threshold for convergence in the scf calculation is 1.0d-10 Ryd. The kmesh is 6\*6\*6 without grid shifting.
   9. The convergence evidence can be seen from the Fig. 1 below.

A picture containing letter

Description automatically generated A picture containing letter

Description automatically generated Chart

Description automatically generated with low confidence

Fig.1 Electronic band structure obtained with different kmesh.

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

scf: 4.36s with 40 cores

bands.1 8.84s

bands.2 14.85s

bands.3 9.15s

band.1 15.50s

band.2 17.83s

band.3 10.16s

* 1. Input files are located at ‘data/1.structure&electronic/scf.in and band\*’

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

2.4641492 0.0000000 0.0000000

0.0000000 2.4641492 0.0000000

0.0000000 0.0000000 2.4641492

Born effective charge

Rb

1.1647523 0.0000000 0.0000000

0.0000000 1.1647523 0.0000000

0.0000000 0.0000000 1.1647523

Br

-1.1647523 0.0000000 0.0000000

0.0000000 -1.1647523 0.0000000

0.0000000 0.0000000 -1.1647523

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

integration mesh: 6\*6\*6

* 1. Convergence evidence

Diagram

Description automatically generated Diagram

Description automatically generatedDiagram

Description automatically generated

Fig.2 Phonon dispersion relation obtained with different kmesh.

* 1. Computational time: 53m27.26s with 40 cores
  2. All input files are located at ‘data/2.harmonic/\*.in’

1. Anharmonic thermal transport
   1. Lattice thermal conductivity v.s. temperature data is stored at ‘data/3.anharmonic/kappa\_vs\_T.csv’
   2. Accumulated lattice thermal conductivity w.r.t mfp is at ‘data/3.anharmonic/ mfp\_kappa.csv’
   3. Accumulated lattice thermal conductivity w.r.t mfp is at ‘data/3.anharmonic/ omega\_kappa.csv’
   4. Scattering rate data is at ‘data/3.anharmonic/sr.csv’
   5. Delta function is represented with adaptive smearing; the integration grid is 24\*24\*24; Symmetry is employed.
   6. Cutoff: 0.926 nm (6th nearest neighbour)
   7. Supercell size: 5\*5\*5
   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. EvenLow temperature w/ isotope (4 data points) takes 5m04s with 40 cores

Low temperature w/ isotope (11 data points) takes 8m43s with 40 cores

High temperature w/ isotope (7 data points) takes 6m58s with 40 cores

EvenLow temperature w/o isotope (4 data points) takes 26m50s with 40 cores

EvenLow temperature w/o isotope (4 data points) 26\*26\* 26 kgrid takes 9m03s with 40 cores

Low temperature w/o isotope (4 data points) takes 9m9s with 40 cores

High temperature w/o isotope (7 data points) takes 10m10s with 40 cores

* 1. All the input files are stored in ‘data/3.anharmonic/inputs’ folder.