Summary note of the phonon olympics entry for AlN

- **Author**: Terumasa TADANO (NIMS)
- **Date**: Feb. 28, 2023.
- **Codes**: VASP 6.2.1 + ALAMODE 1.4.2 (some new features of dev branch are also tested)
- **Compilers**: Intel Compiler version 20.0.2.254 + Intel MKL
- **Compile flags**: `-O2` for ALAMODE, `-O2 -xHOST` for VASP
- **MPI library**: HPE MPI 2.21
- **Computer Resource**: NIMS simulator (Intel Xeon Platinum 8268 24core 2.9 GHz x 2 / node)

1. Structure - summary

The calculations were performed using `VASP` code with the following input parameters:

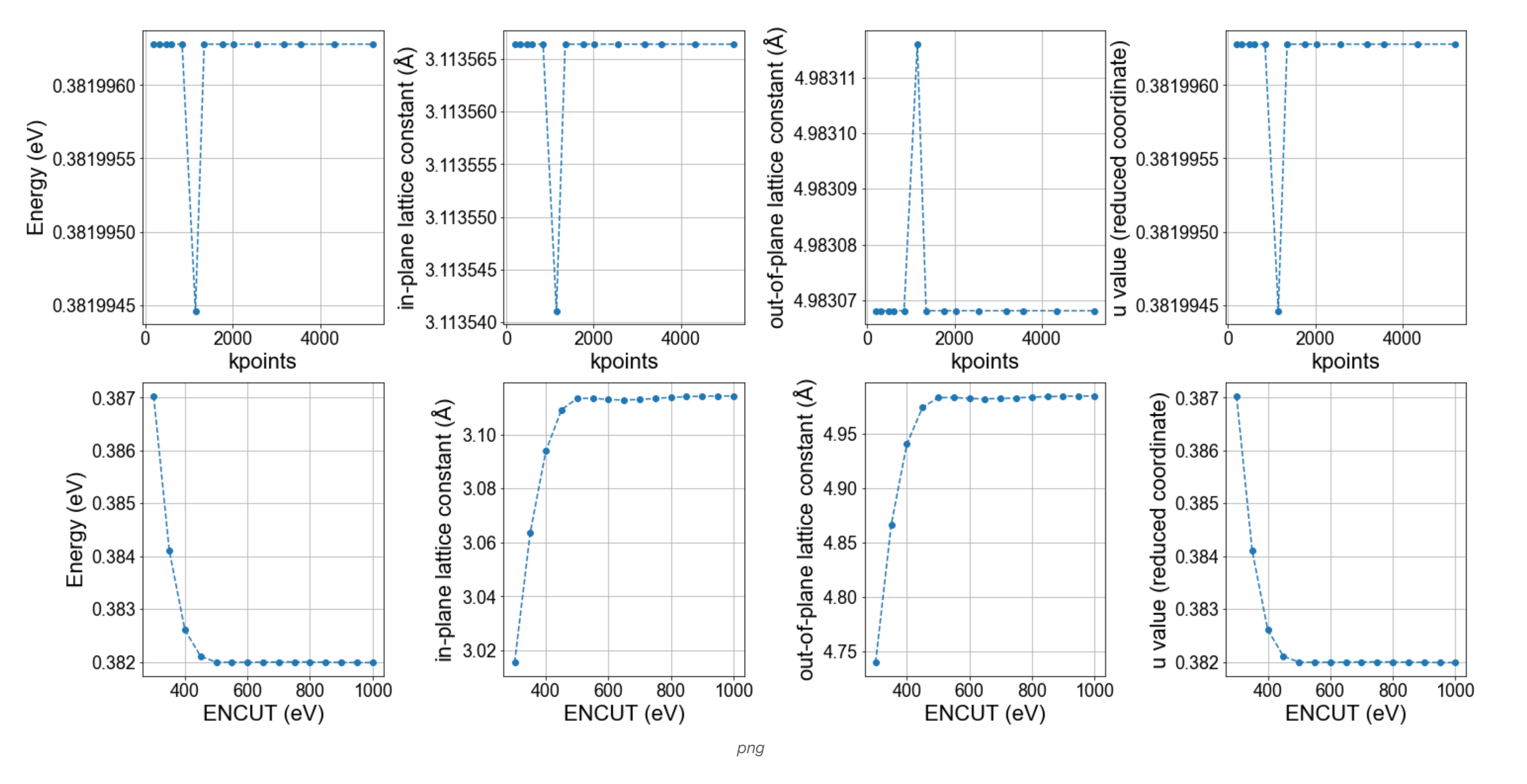
```
PREC = Accurate
ENCUT = 550
EDIFF = 1.0e-8
EDIFFG = -0.5e-3
ISMEAR = 0
SIGMA = 0.05
ALGO= Normal
LREAL = .FALSE.
ADDGRID = .TRUE.
LWAVE = .FALSE.
LCHARG = .FALSE.
ICHARG= 2
ISTART=0
NELM=200

NPAR = 12
KPAR = 4
ISIF = 3
IBRION = 1
NSW = 100
POTIM = 0.1

GGA = PS
LAPSH = .True.
```

As shown in the tables and figures below, the lattice constants appear to reach convergence at the 12x12x8 k points and `ENCUT=550`.

- **ENCUT = 550**
- **12x12x8 k points for primitive**
- **a = 3.114 Angstrom**
- **c = 4.983 Angstrom**
- **u = 0.382**



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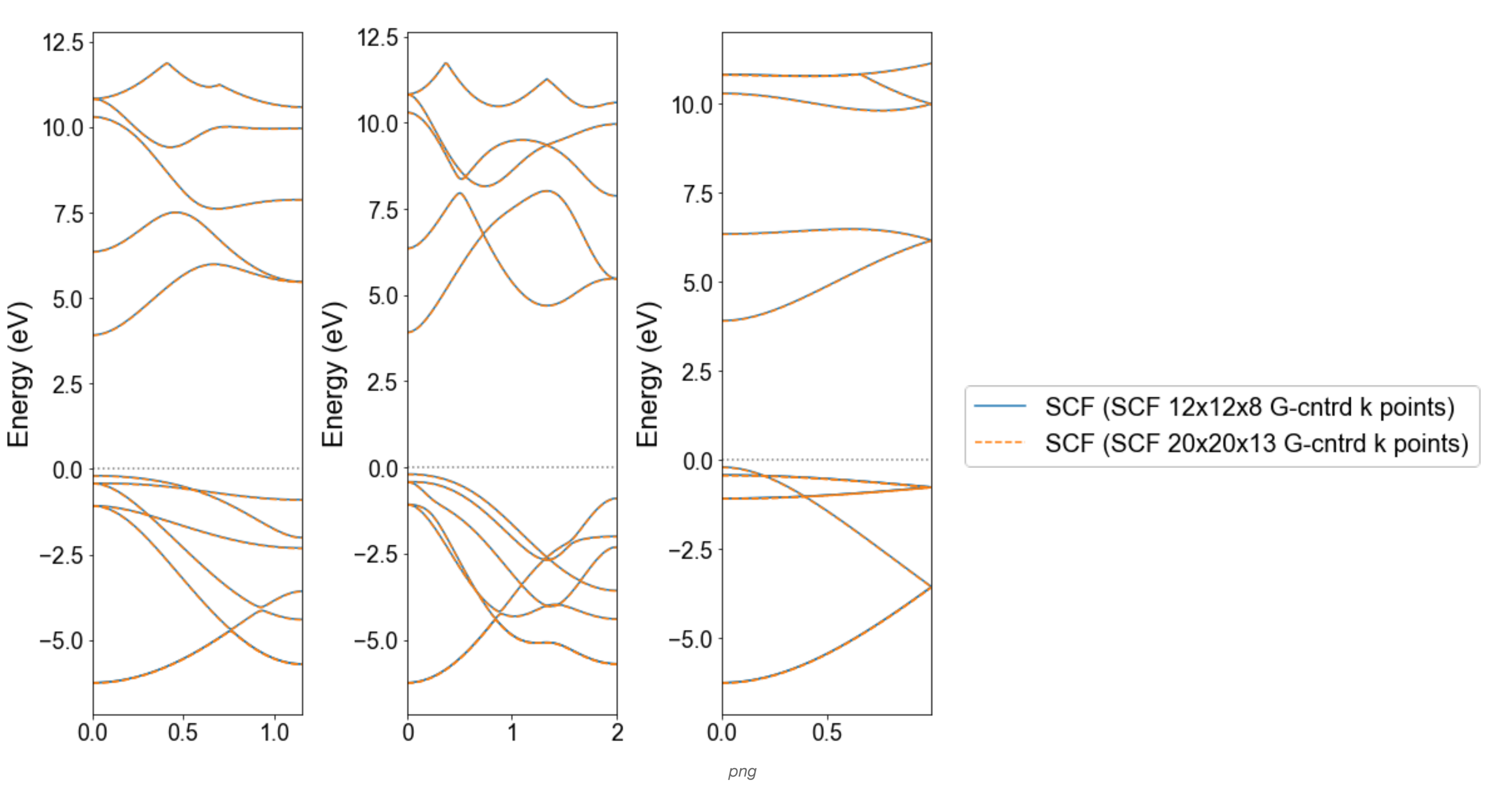
2. Electronic - summary

The electronic band dispersion obtained from the 12x12x8 k points agrees well with the result obtained from the denser 20x20x13 k points. So, we conclude that 12x12x8 kpoints was accurate enough.



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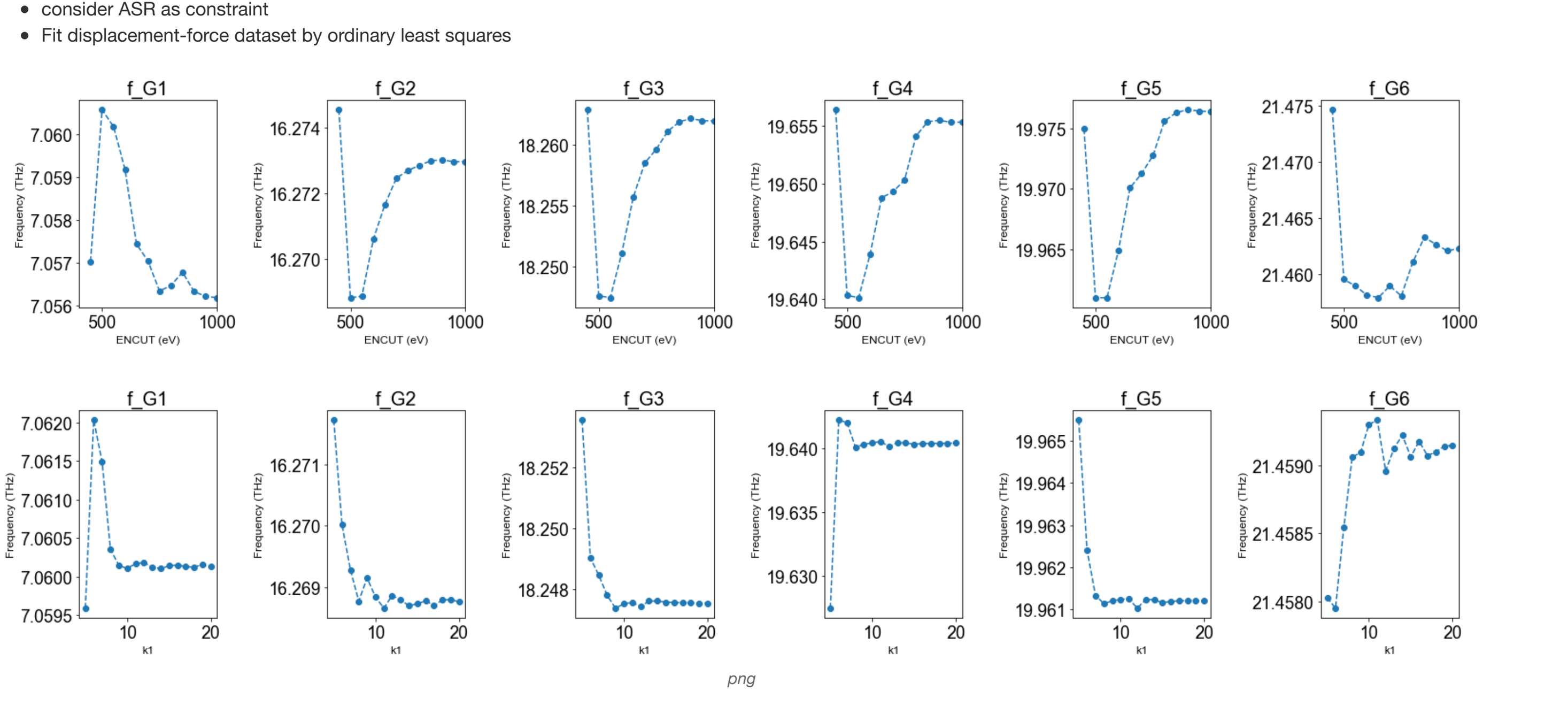
3.1 Harmonic - convergence at G and M points

The phonon frequencies at Gamma (0,0,0) points are calculated using the following conditions:

- primitive cell (4 atoms)
- displacement magnitude : 0.01 Angstrom
- make full use of symmetry (permutation, space group)
- consider ASR as constraint
- Fit displacement-force dataset by ordinary least squares



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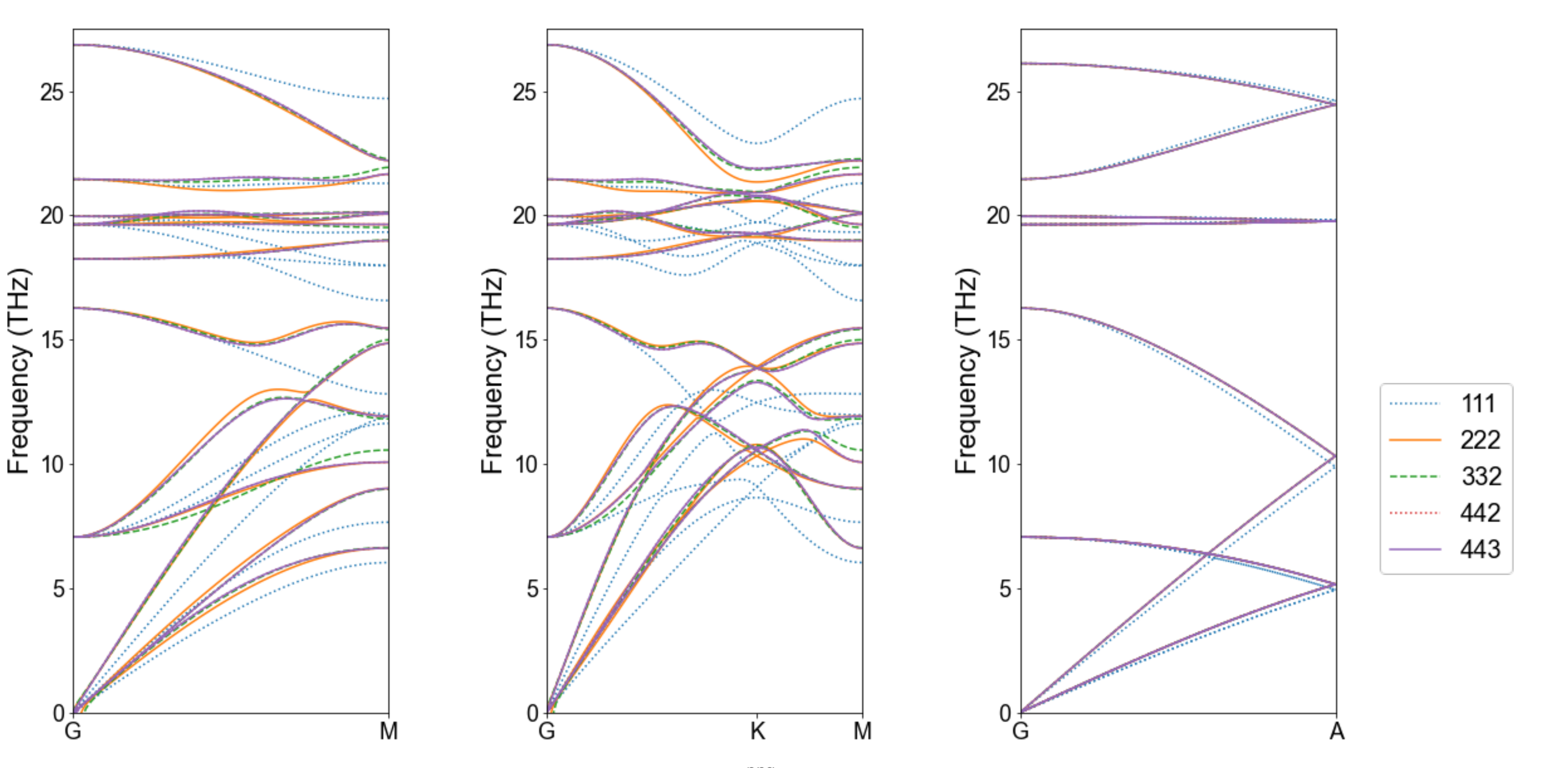
3.2 Harmonic - convergence of dispersion

To examine the convergence of phonon dispersion curves, we have performed phonon calculations using various supercells and k points as summarized below:

	Supercell (SC) size	# atoms in SC	ENCUT	k mesh style	k mesh	k mesh shift	Core hours	magnitude of\ndisplacement (Ang.)
0	111	4	550.0	Gamma	[12, 12, 8]	[0.0, 0.0, 0.0]	1.441013	0.01
1	222	32	550.0	Gamma	[6, 6, 4]	[0.0, 0.0, 0.0]	17.772160	0.01
2	332	72	550.0	Gamma	[4, 4, 4]	[0.0, 0.0, 0.0]	48.105067	0.01
3	442	128	550.0	Gamma	[3, 3, 4]	[0.0, 0.0, 0.0]	128.332427	0.01
4	443	192	550.0	Gamma	[3, 3, 3]	[0.0, 0.0, 0.0]	233.681227	0.01

The results are plotted in the **figure below.**



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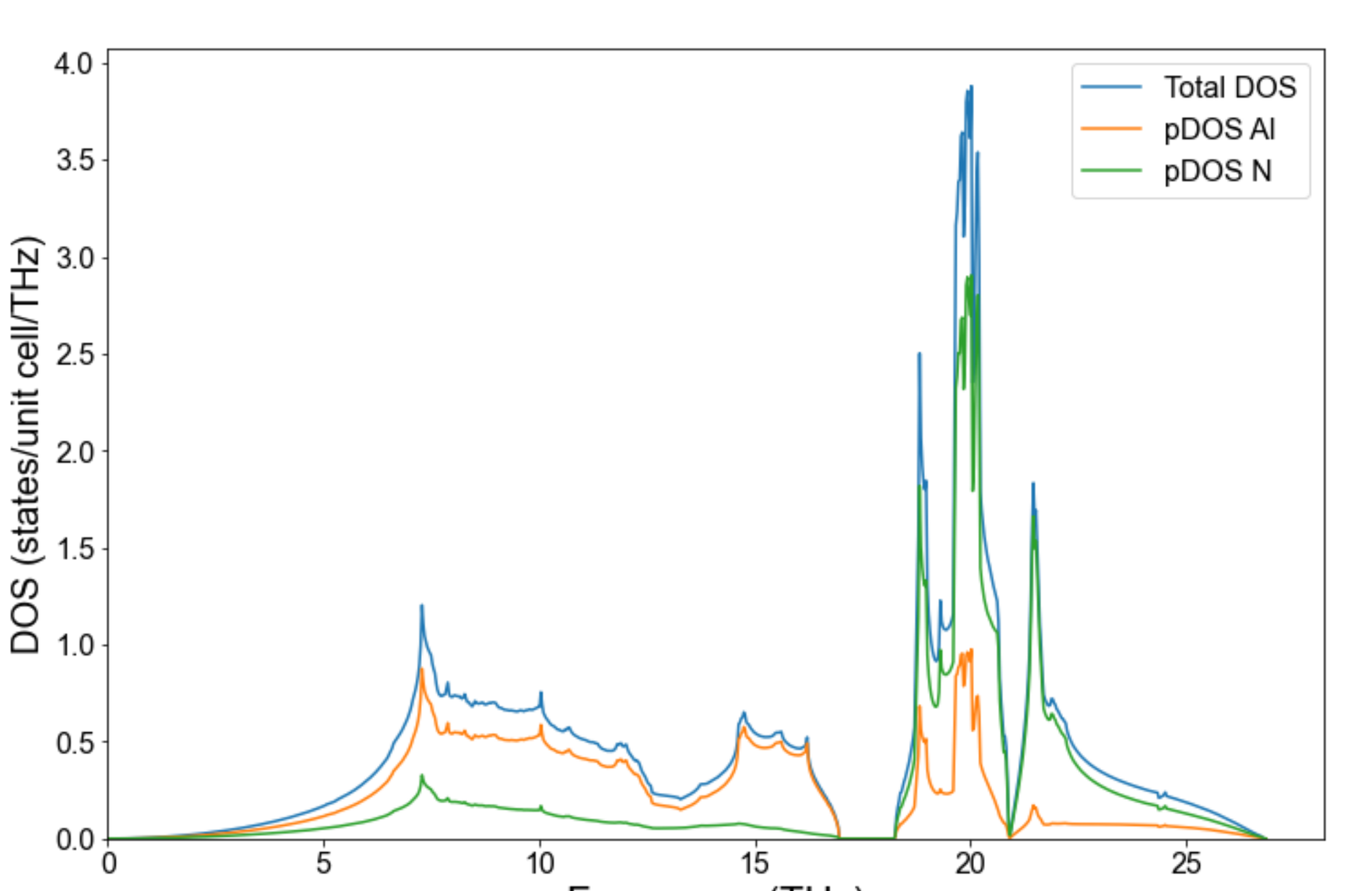

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4.1 Anharmonic - convergence w.r.t. cutoff radius, supercell size, and the size of the training data

The result of the convergence check with respect to the cutoff radius for the third-order IFC is shown in the table and figures below.

The force constants are calculated with the following methods:

- Random displacements of all atoms with magnitude of 0.03 Ang.
- Full space group symmetry considered
- Impose ASR as constraints
- Estimate third-order IFCs by ordinary least squares, LASSO and adaptive-LASSO (optional)
- **When fitting the third-order IFCs, the second-order IFCs are fixed to the values obtained in the step 3.**

The thermal conductivity calculations are performed with the following conditions:

- 13x13x9 q points
- Use space group symmetry for reducing sampling q points and triplets (q, q‘, q”)
- Tetrahedron method (`ISMEAR = -1`) for delta function evaluation
- Atomic mass : 26.9815384 au (Al), 14.003074 au (N)
- RTA
- no ph-iso scattering, no ph-boundary effects
- Phonon group velocity is evaluated as $\boldsymbol{v}_{\boldsymbol{q}j} \approx (\omega_{\boldsymbol{q}+\Delta\boldsymbol{q}j} - \omega_{\boldsymbol{q}-\Delta\boldsymbol{q}j})/2\Delta\boldsymbol{q}$ where $\Delta\boldsymbol{q}$ is a small value (~0.001).
- Nonanalytic correction with Ewald method.

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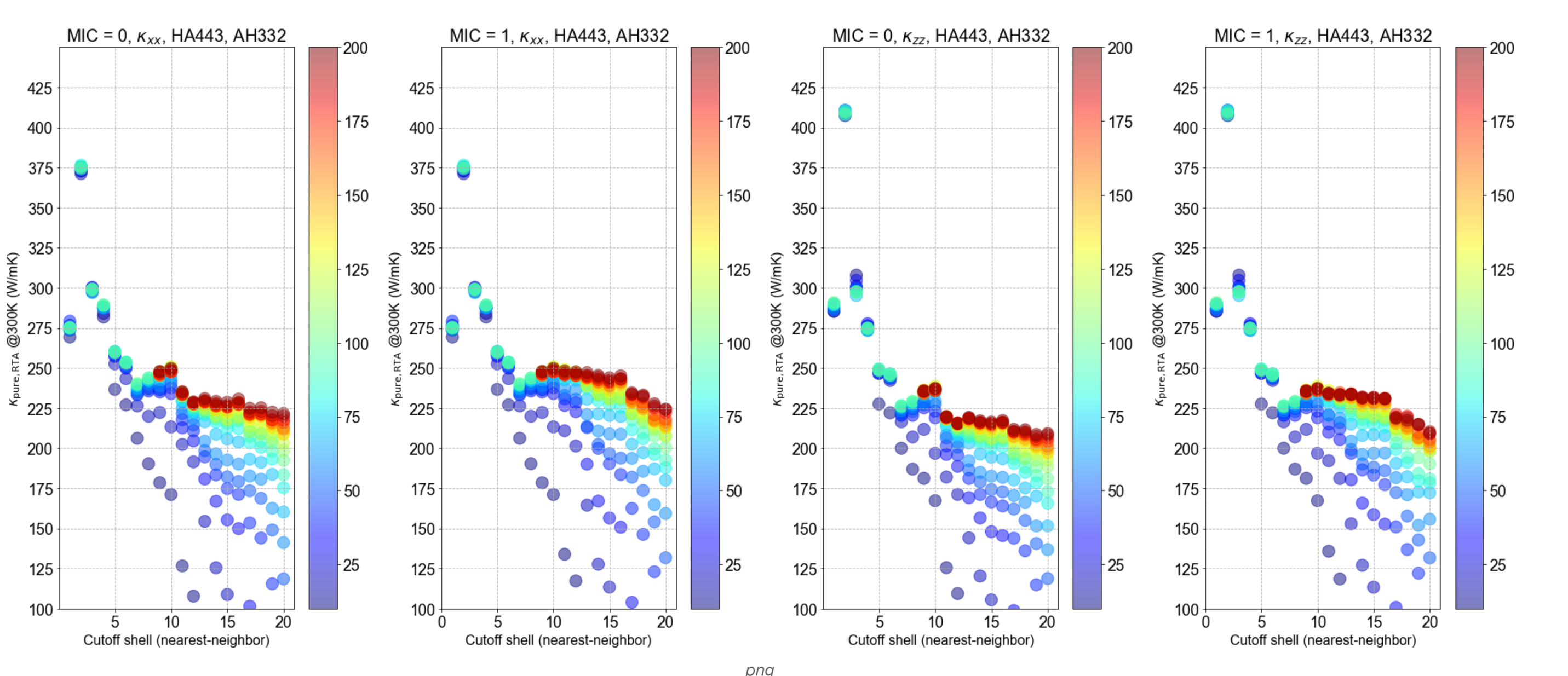

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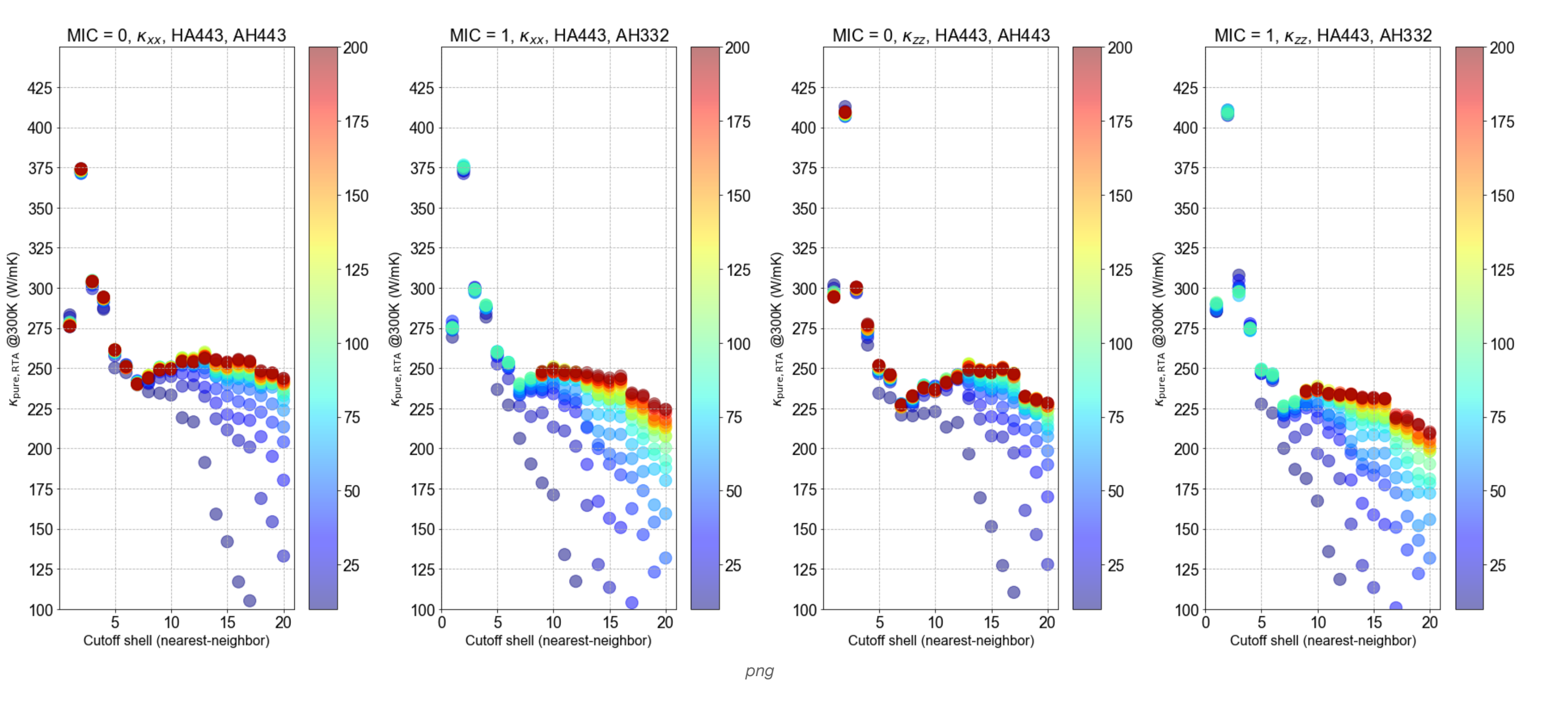

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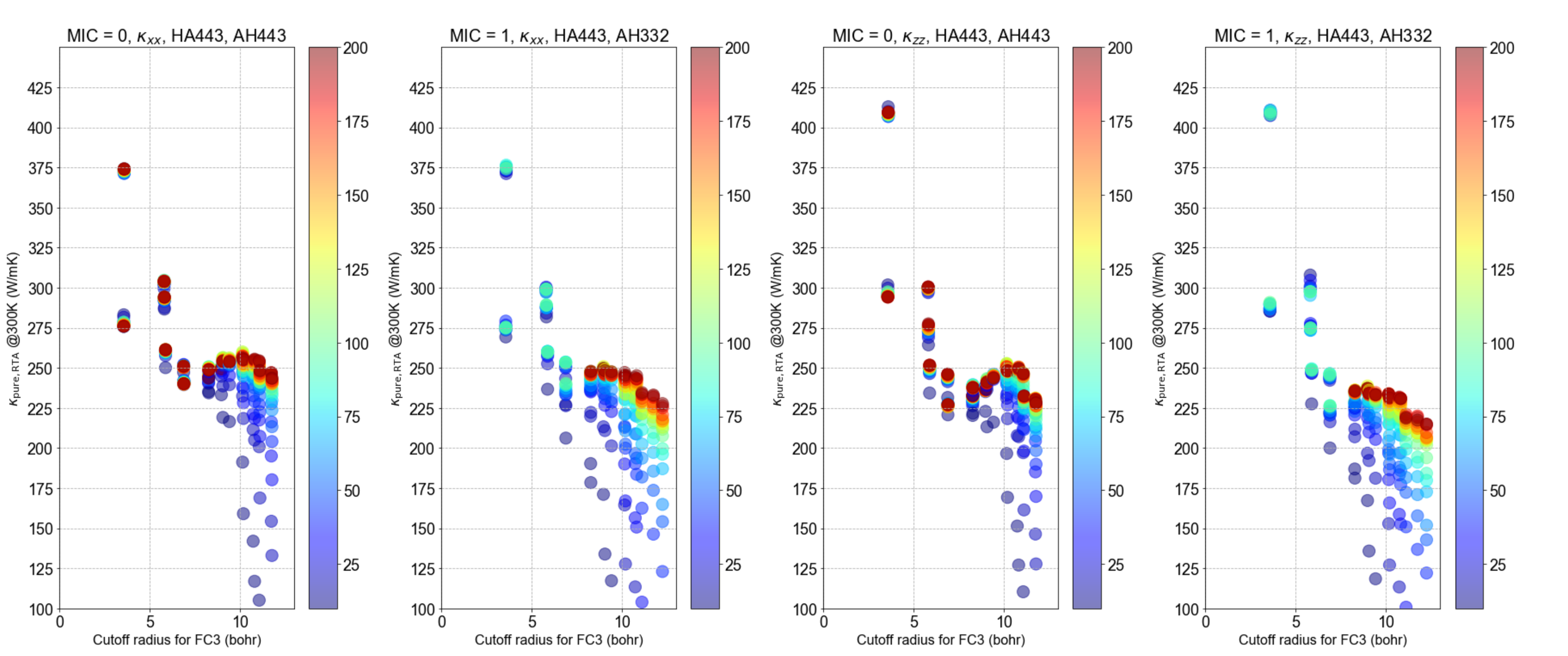

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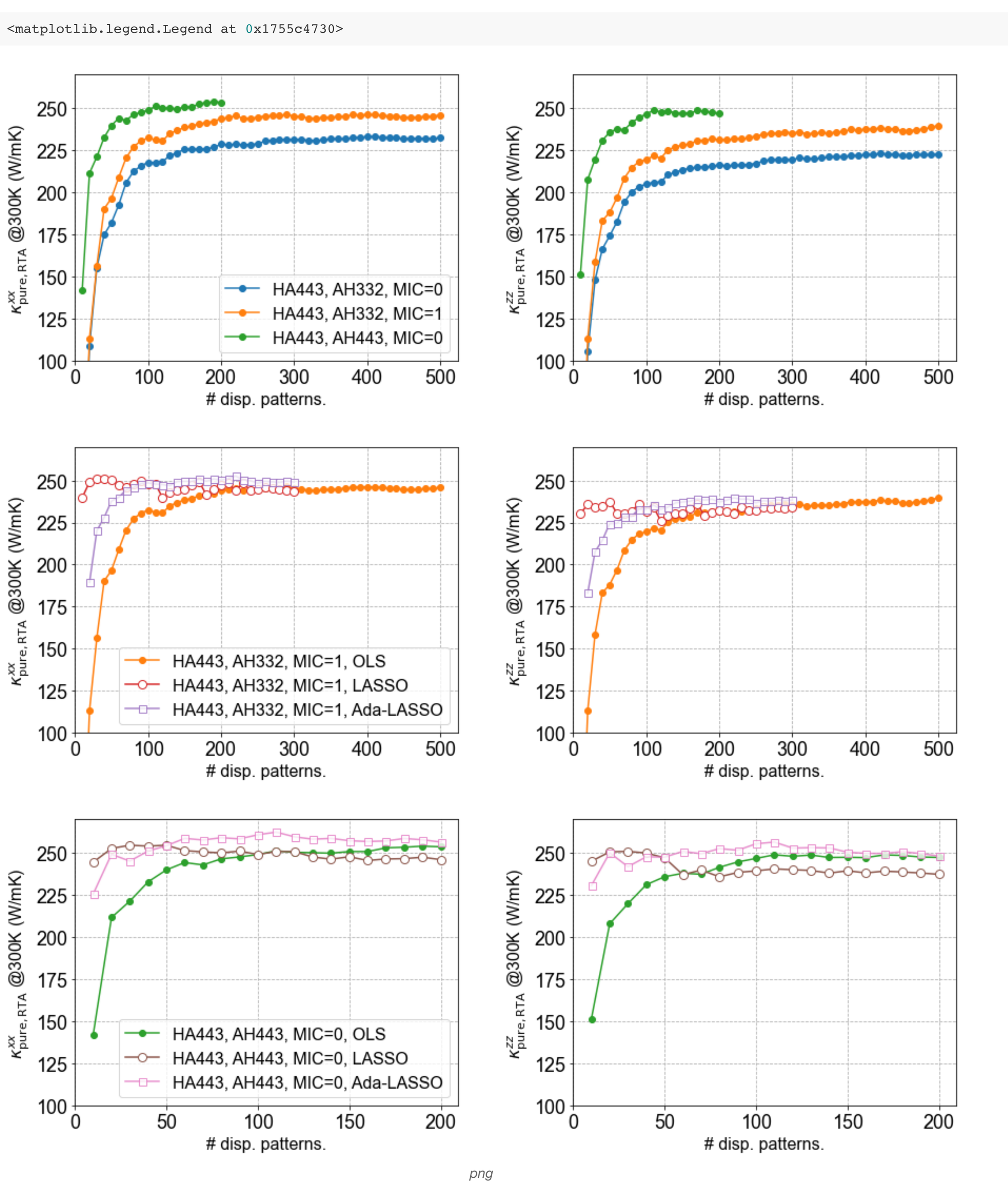

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4.2 Anharmonic - convergence w.r.t. q mesh

The convergence of κ_{L} with respect to the q point density was examined using the following computational conditions:

- 4x4x3 supercell for second-order and third-order IFCs
- RTA
- No isotope scattering

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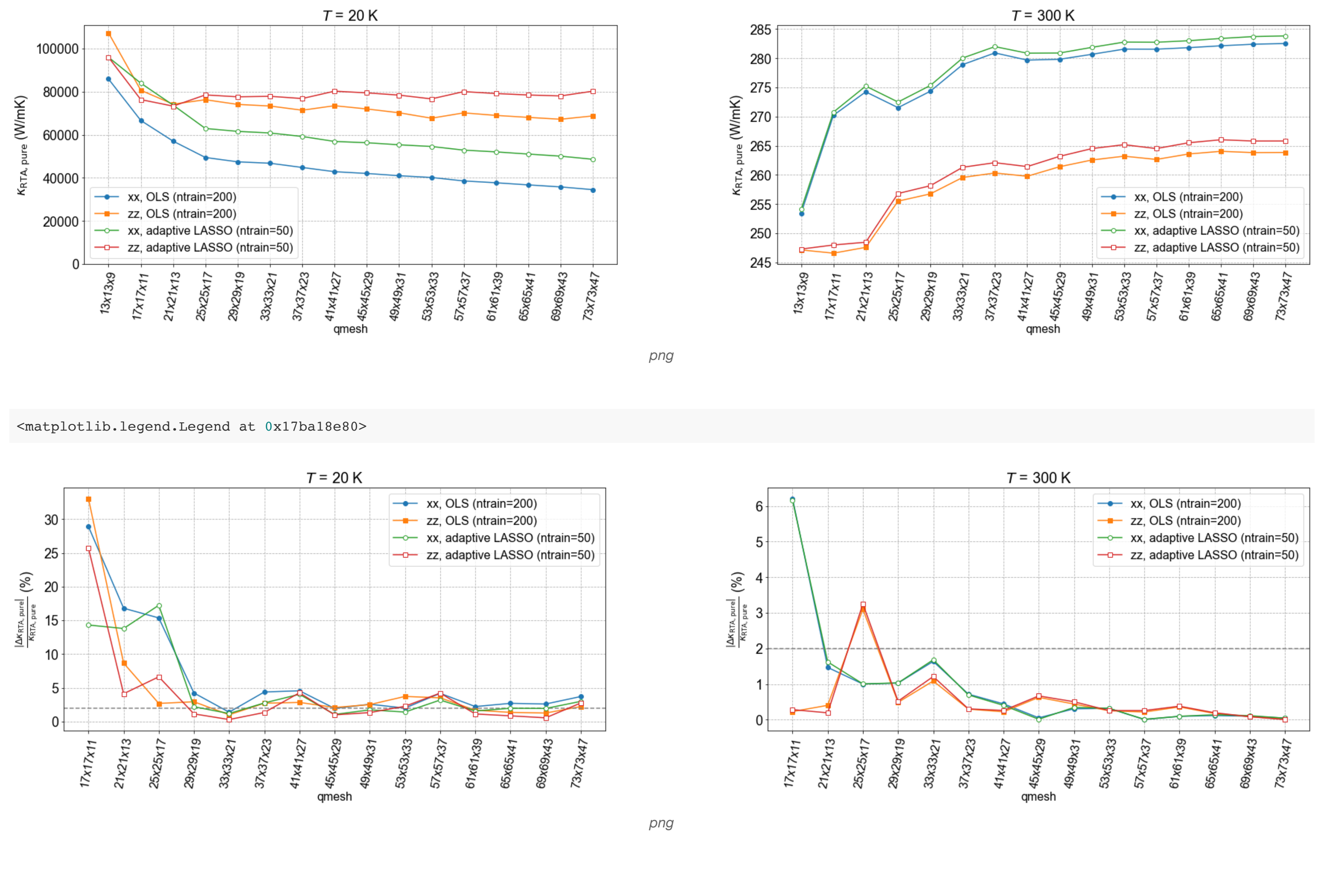

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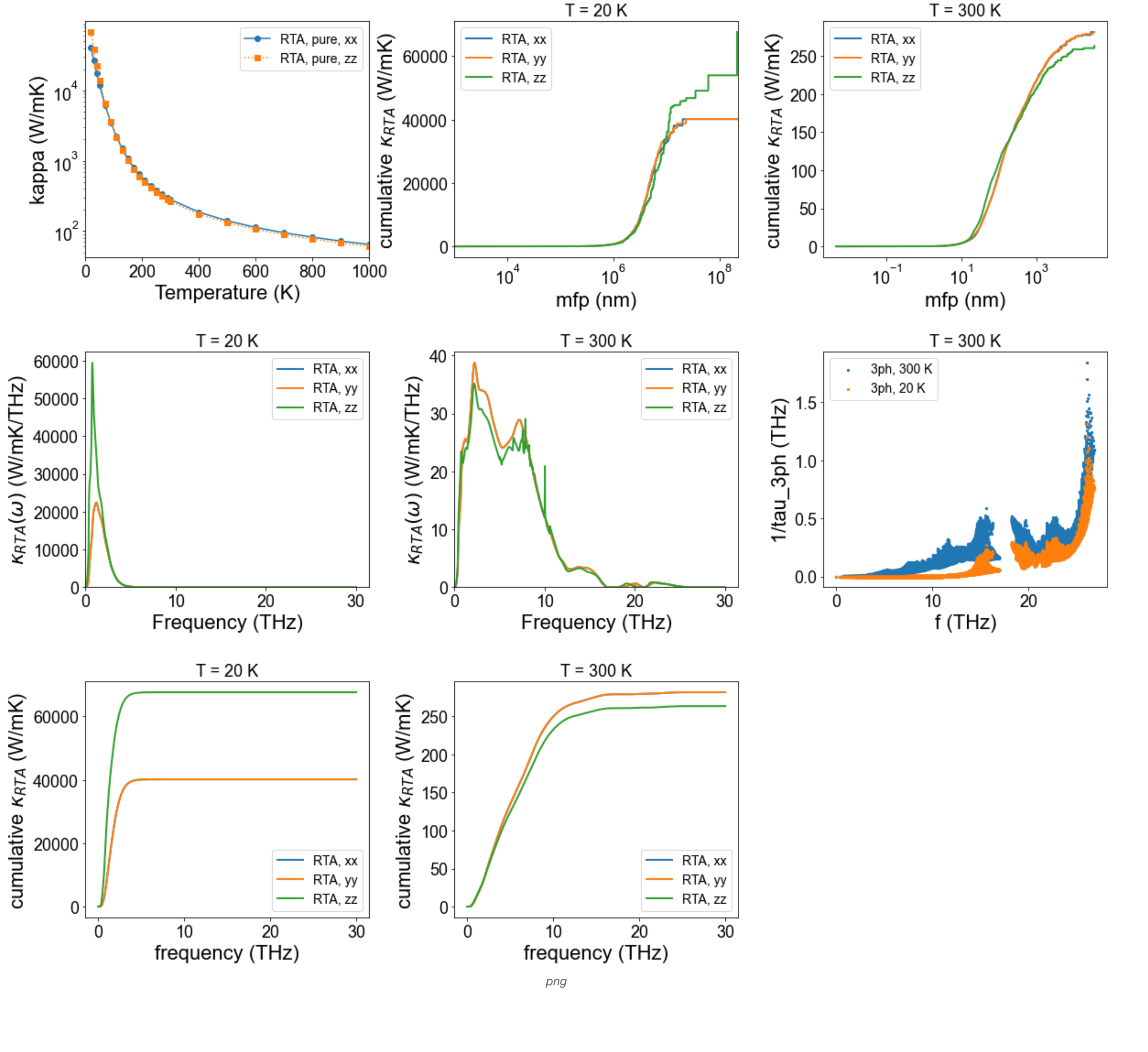
4. Anharmonic - production run

After checking the convergence of kappa w.r.t. various parameters, I have chosen the following set of parameters for the production calculation.

- Lattice constant (Ang.) : a = 3.1135, c = 4.9831
- ENCUT = 550
- SC for IFC2: `443`
- SC for IFC3: `443`
- Cutoff radius for IFC3 (bohr): 10.74 (includes up to 15NN shells)
- 55x55x33 q points
- tetrahedron method for delta function
- Mass of Al : 26.9815384 au
- Mass of N : 14.003074 au
- temperature step: 10 K

The results of the production calculation are shown in the following tables/figures.



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