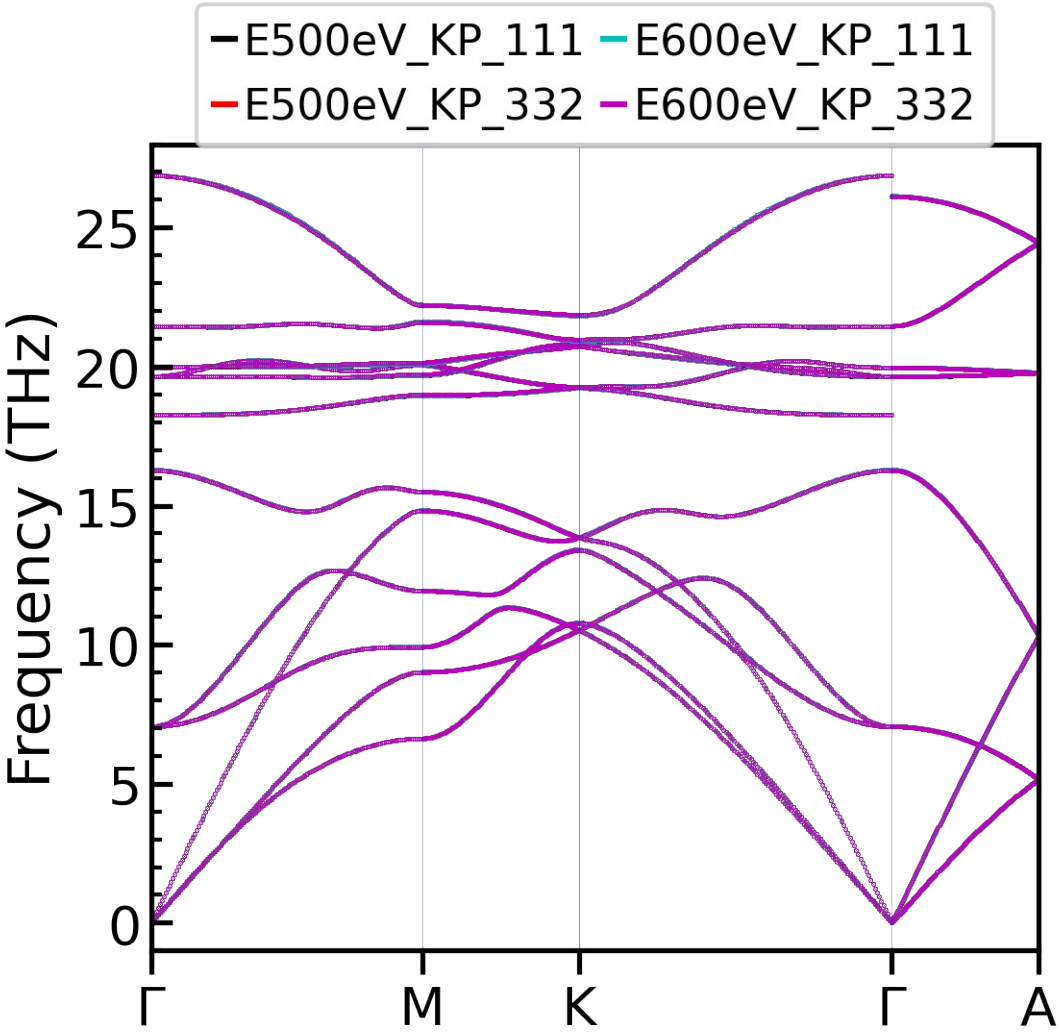
Lattice thermal conductivity for wurtzite AlN in phono3py

Relaxed a = 3.113 Ang and c = 4.9821 Ang

Supercell 5x5x2 : Finite difference method

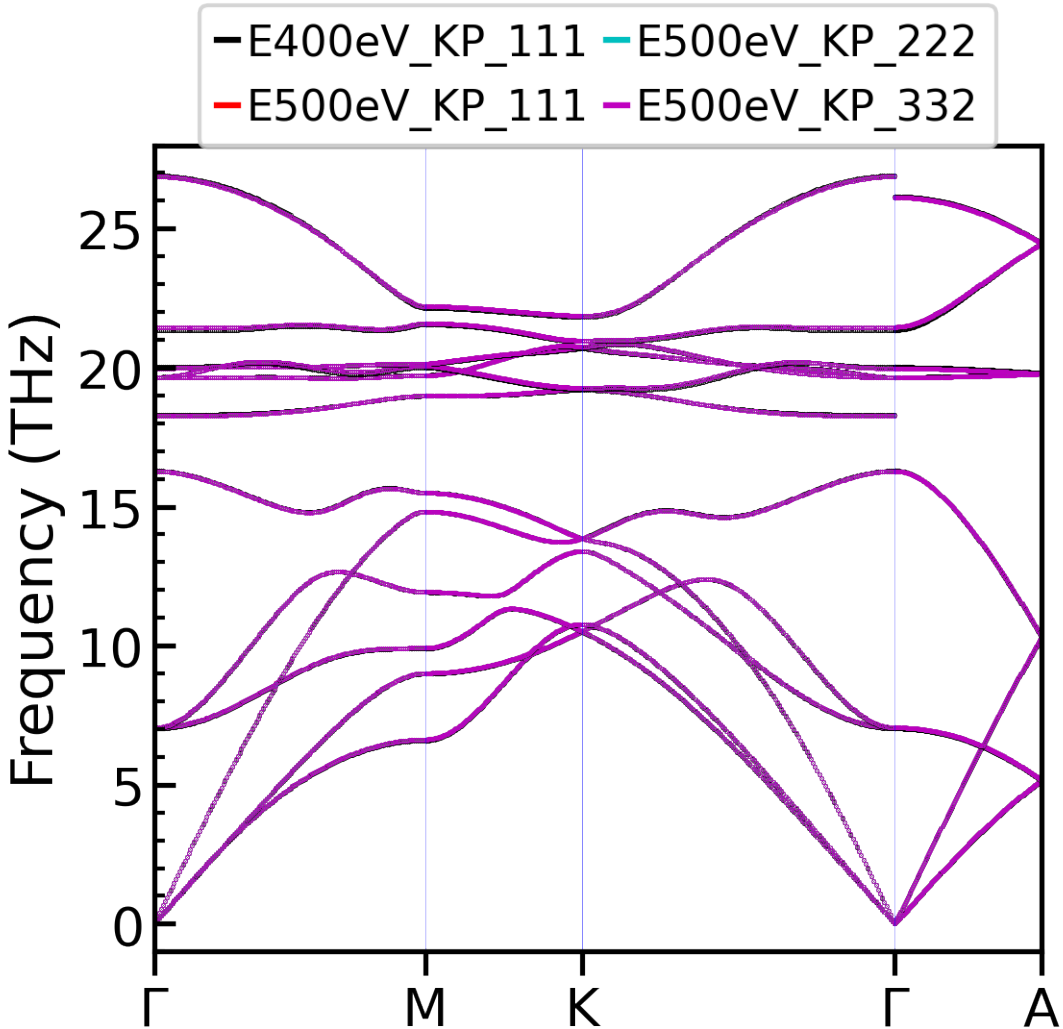


- E refers to energy cutoff, KP refers to
- K-points grid used in force calculations
- within VASP.

- ALM is used to generate force constants.

- For Ecut 500 eV, and higher phonons frequency seems converge.

Supercell 5x5x3 : Finite difference method

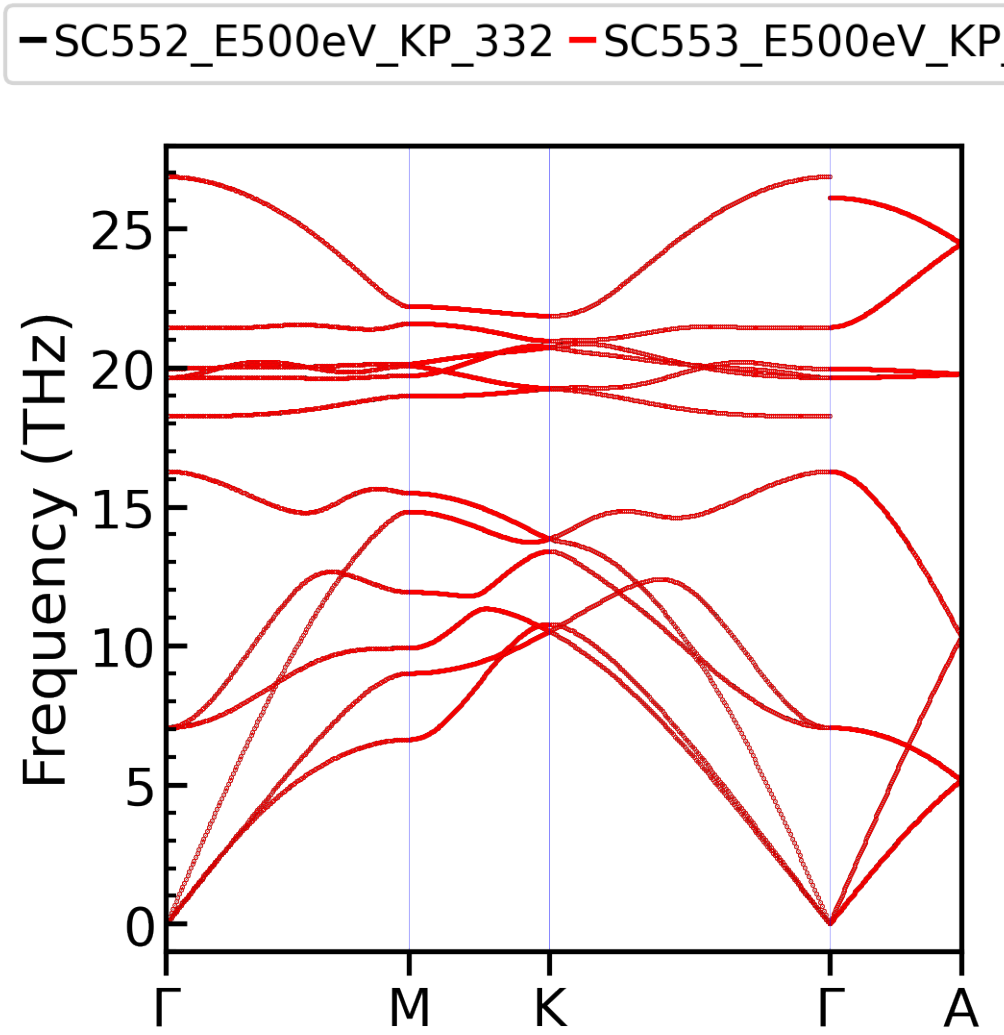


- E refers to energy cutoff, KP refers to
- K-points grid used in force calculations
- within VASP.

- ALM is used to generate force constants.

- For Ecut 500 eV, and higher phonons frequency seems converge.

Comparison of different super cell sizes :Finite difference method



- Sc refers to supercell size, E refers to energy cutoff, KP refers to K-points grid used in force calculations within VASP.
- ALM is used to generate force constants.
- For Ecut 500 eV, and higher phonons frequency seems converge.
- For supercell 5x5x2 and 5x5x3 phonons are similar
- **From here we take 5x5x3 as best supercell for 2nd order Ifcs computation**

3rd order IFCs

Here various combination of supercell and K-points are tested

- 3x3x2 supercell with Gamma point only
- 3x3x2 supercell with Kpoints 3x3x3 with G-centered mesh
- 3x3x2 supercell with Kpoints 2x2x2 with k-mesh shifted by (0,0,1/2)
- 4x4x2 supercell with Gamma point only
- 4x4x2 supercell with 3x3x3 with G-centered mesh
- 5x5x3 supercell with Gamma point only

- **Here all possible interactions in the super-cell are included.**
-
- **Both 2nd and 3rd order IFCs are computed within finite difference method**

Lattice thermal conductivity at 300K

Using tetrahedron method, without phonon-isotope scattering, non-analytical correction method: X. Gronze

A	B	C	D	E	F	G
2nd Ifcs	**3rd IFCs**	**Q-mesh**	**Direct sol (300K)**		**RTA (300K)**	
			kxx	**kzz**	**kxx**	**kzz**
552-KP-553	**3x3x2 Gamma point-only**	31x31x17	278.88	259.14	247.797	222.483
552-KP-553	**332-KP333-G-centered**	31x31x17	283.927	262.45	252.287	226.04
552-KP-553	**332-KP222-(0,0,1/2) shifted**	31x31x17	283.886	262.45	252.234	226.007
552-KP-553	**442-Gamma point-only**	31x31x17	290.152	267.851	259.406	231.23
553-KP-332	**3x3x2 Gamma point-only**	31x31x17	279.88	267.908	248.416	228.276
553-KP-332	**332-KP333-G-centered**	**31x31x17**	**285.048**	**271.262**	**252.992**	**231.947**
553-KP-332	**332-KP222-(0,0,1/2) shifted**	**31x31x17**	**285.002**	**271.261**	**252.936**	**231.91**
553-KP-332	**442-Gamma point-only**	31x31x17	291.211	276.495	260.105	237.201
553-KP-332	**442-KP-222**	31x31x17	291.17	276.812	259.217	237.179
553-KP-332	**553-Gamma point-only**	31x31x17	283.952	263.79	251.339	225.841