**Aluminum Nitride (AlN)**

*Space group*: P63mc, 186, wurtzite

*Lattice vectors*: *R*1 = (*a*, 0, 0); *R*2 = (-*a*/2, *a*×*sqrt*[3]/2, 0); *R*3 = (0, 0, *c*)

*Atom positions*: Al1 = (0, *a*/*sqrt*[3], 0); Al2 = (*a*/2, *a*/(2×*sqrt*[3]), *c*/2); N1 = (0, *a*/*sqrt*[3], *u×c*); N2 = (*a*/2, *a*/(2×*sqrt*[3]), (1/2+*u*)×*c*). Note that *u* is an internal degree of freedom.

[crystal: Al1 = (1/3, 2/3, 0); Al2 = (2/3, 1/3, 1/2); N1 = (1/3, 2/3, *u*); N2 = (2/3, 1/3, 1/2*+u*)]

*Isotopes*: **consider isotopically pure** (Al is pure and N is relatively pure)

*DFT*: PBEsol PAW

QE - Al.pbesol-n-kjpaw\_psl.1.0.0.UPF and N.pbesol-n-kjpaw\_psl.1.0.0.UPF

VASP - standard version with sol flag

**Checklist** (*all data should be reported for the 4-atom primitive cell*)

***Structure***

* Converged relaxed ‘temperature (T)=0’ lattice constants *a*, *c*, and *u* (target accuracy < 0.01 Å) where *a* is the in-plane lattice parameter, *c* is the cross-plane parameter, and *u* is the internal degree of freedom between AlN formula units

- Three values with 3 significant figures: X.XX

* Methods / convergence criteria

- Energy / force thresholds

* Other notes / cpu hours (*e.g., multiple relaxations, compilers, hardware*)
* All input files to run fully converged calculations (*e.g., qe.scf.in, POSCAR*)

***Electrons***

* Converged electron band dispersion (target accuracy < 0.1 eV for Γ point energies)

- Numerical data: normalized wavevectors (q) and band energies (E): top 6 valence bands and 6 conduction bands (excel or text file)

- q in units of π/*a* for in-plane and π/*c* for cross-plane; E in eV

- 2 in-plane segments: Γ→M, Γ→K→M, and 1 cross plane segment: Γ→A, evenly divided with ~100 q points per segment

- 3 files, one for each segment. For each scaled q from 0 to 1 list (~100 rows): q, E1, E2, E3, E4, E5, E6, E7, E8, E9, E10, E11, E12

* Methods / convergence criteria

- Thresholds/ Integration mesh / grid shifting

* Other notes / cpu hours
* All input files to run fully converged calculations

***Harmonic***

* Converged dispersion (target accuracy < 0.1 THz for Γ point frequencies)

- Numerical data: normalized wavevectors (q) and frequencies (f) for 12 polarizations (*j*) (excel or text file)

- q in units of π/*a* for in-plane and π/*c* for cross-plane; f in THz (f=ω/2π)

- 2 in-plane segments: Γ→M, Γ→K→M, and 1 cross-plane segment Γ→A, evenly divided with ~100 q points per segment

- 3 files, one for each segment. For each scaled q from 0 to 1 list (~100 rows): q, f1, f2, f3, f4, f5, f6, f7, f8, f9, f10, f11, f12

- **phonon density of states**

* Converged harmonic interatomic force constants (IFCs)

- Standard format for code used (*e.g.*, QE, Phonopy)

- Will be supplied as supplemental material upon publication

* Long range Coulomb corrections
* Dielectric matrix (1 matrix)
* Born effective charge matrices (4 matrices)
* Method of long-range Coulomb corrections
* Methods / convergence criteria

- Thresholds

- Supercell size / integration mesh

- Symmetries / irreducibility / number of calculations (*linked to cpu hours below*)

- Post-processing (*e.g., enforce invariance constraints*)

* Evidence of converged dispersion

- Dispersions with varying supercell sizes and integration meshes

* Other notes / cpu hours (*e.g., accuracy vs cpu cost, shifted meshes*)
* All input files to run fully converged calculations

***Anharmonic thermal transport***

* Six converged T-dependent thermal conductivities (*k*) (target accuracy <2% difference between successive grids): isotopically pure with full BTE solution (*kpure,full*), and isotopically pure with RTA (*kpure,RTA*) for two in-plane directions (*x* and *y*) and one cross-plane direction (*z*). If only RTA available, then only *kpure,RTA*.

- Do not include boundary scattering, even at low T. We want to see how the codes behave at low T without this extrinsic scattering.

- Numerical data: T (K) and *k* (W/m/K) in range 20K < T < 1000K (excel or text file)

- For 20K ≤ T ≤ 50K increments of 10K (4 data points); for 50K < T ≤ 300K increments of 25K (10 data points); for 300K < T ≤ 1000K increments of 100K (7 data points).

- 1 file with T from 20K to 1000K list (21 rows): T, *kpure,full*, *kpure,RTA*

* Accumulated T=20K and T=300K *kacc* vs frequency (1 curve for each T) for converged *kpure,RTA*
* Accumulated T=20K and T=300K *kacc* vs mean free path (mfp) for converged *kpure,RTA*: 3 curves for each T, one for each in-plane (mfp*x*=|*vx*×lifetime| and mfp*y*=|*vy*×lifetime|in nm) and one for cross-plane (mfp\_cross=|*vz*×lifetime| in nm).

- Numerical data for each mode (q, *j*) sampled in the Brillouin zone integration: f (THz), mfp (nm), mode contribution to *k* (W/m/K) for *kpure,RTA*

- 2 files (excel or text; one for each T) with row for each mode (q, *j*): f, mfp *x*, mfp *y*, and mfp *z*, mode contribution to *k*

* RTA T=300K three-phonon scattering rates (1/*τ3ph*)

- Numerical data: f (THz), 1/*τ3ph* (THz=1/ps)

- 1 file (excel or text) with row for each mode (q, j): f, 1/*τ3ph*

* Converged third-order anharmonic IFCs

- Standard format for code used

- Will be supplied as supplemental material upon publication

* Methods / convergence criteria: thermal conductivity

- Delta function representation (*with details; e.g., adaptive smearing, cutoff*)

- Integration grid

- Symmetries used

* Methods / convergence criteria: anharmonic IFCs

- Cutoff radius, supercell size, integration mesh, thresholds, displacement parameter for supercell derivatives

- Post-processing

* **Evidence of converged *k* at T=20K and T=300K (Do not go to extreme numerical cost for T=20K. If convergence seems not possible please consult Alan and Lucas).**

- Varying integration meshes

- Target accuracy <2% difference between successive grids

* Other notes / cpu hours
* All input files to run fully converged calculations