Aluminum Nitride (AlN)

Space group: $P6_3mc$, 186, wurtzite
Lattice vectors: $R_1 = (a, 0, 0)$; $R_2 = (-a/2, a \times sqrt[3]/2, 0)$; $R_3 = (0, 0, c)$
Atom positions: $Al_1 = (0, a/sqrt[3], 0)$; $Al_2 = (a/2, a/(2 \times sqrt[3]), c/2)$; $N_1 = (0, a/sqrt[3], u \times c)$; $N_2 = (a/2, a/(2 \times sqrt[3]), (1/2+u) \times c)$. Note that u is an internal degree of freedom.
[crystal: $Al_1 = (1/3, 2/3, 0)$; $Al_2 = (2/3, 1/3, 1/2)$; $N_1 = (1/3, 2/3, u)$; $N_2 = (2/3, 1/3, 1/2+u)$]
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, E_1, E_2, E_3, E_4, E_5, E_6, E_7, E_8, E_9, E_{10}, E_{11}, E_{12}
- 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 ($f=\omega/2\pi$)
  - 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, f_1, f_2, f_3, f_4, f_5, f_6, f_7, f_8, f_9, f_{10}, f_{11}, f_{12}
    - **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 ($k_{pure,full}$), and isotopically pure with RTA ($k_{pure,RTA}$) for two in-plane directions (x and y) and one cross-plane direction (z). If only RTA available, then only $k_{pure,RTA}$.
    - 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, $k_{pure,full}$, $k_{pure,RTA}$
- Accumulated T=20K and T=300K k_{acc} vs frequency (1 curve for each T) for converged $k_{pure,RTA}$
- Accumulated T=20K and T=300K k_{acc} vs mean free path (mfp) for converged $k_{pure,RTA}$: 3 curves for each T, one for each in-plane ($mfp_x=|v_x \times lifetime|$ and $mfp_y=|v_y \times lifetime|$ in nm) and one for cross-plane (mfp_cross=$|v_z \times lifetime|$ 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 $k_{pure,RTA}$
    - 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 ($1/\tau_{3ph}$)
    - Numerical data: f (THz), $1/\tau_{3ph}$ (THz=1/ps)
    - 1 file (excel or text) with row for each mode (q, j): f, $1/\tau_{3ph}$

- 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