**kkGermanium**

*Space group*: Fd-3m, 227

*Lattice vectors*: *R*1 = (-*a*/2, 0, *a*/2); *R*2 = (0, *a*/2, *a*/2); *R*3 = (-*a*/2, *a*/2, 0)

*Atom positions*: Ge1 = (0, 0, 0); Ge2 = (*a*/4, *a*/4, *a*/4)

*Isotopes*: 20.38% 70Ge (69.924 amu); 27.31% 72Ge (71.922 amu); 7.76% 73Ge (72.923 amu); 36.72% 74Ge (73.921 amu); 7.83% 76Ge (75.921 amu)

*DFT*: Use VASP, QE, or both. PBEsol PAW, no *d* states in valence   
(QE: Ge.pbesol-n-kjpaw\_psl.1.0.0.UPF; VASP: standard version with sol flag)

*Warning: DFT may give metallic. May need to check convergence with electronic smearing.*

**Checklist** (*all data should be reported for the 2-atom primitive cell*)

***Structure***

* ~~Converged relaxed ‘temperature (T)=0’ lattice constant~~ *~~a~~* ~~(target accuracy < 0.005 Å)~~

- Single value with 4 significant figures: X.XXX

* ~~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.sc.in, POSCAR~~*~~)~~

***Electrons***

* ~~Converged electron band dispersion (target accuracy < 0.1 eV for Γ/X/L frequencies)~~

- Numerical data: normalized wavevectors (q) and band energies (E): 4 valence bands and 6 conduction bands (excel or text file)

- q in units of 2π/*a* and f in eV

- 3 segments: Γ→X, Γ→K→X, and Γ→L 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

* ~~Methods / convergence criteria~~

- Thresholds/ Integration mesh / grid shifting

* ~~Evidence of converged band structure~~

- Band structure with varying integration meshes

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

***Harmonic***

* ~~Converged dispersion (target accuracy < 0.1 THz for Γ/X/L frequencies)~~

- Numerical data: normalized wavevectors (q) and frequencies (f) for 6 polarizations (*j*) (excel or text file)

- q in units of 2π/*a* and f in THz (f=ω/2π)

- 3 segments: Γ→X, Γ→K→X, and Γ→L 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

* ~~Converged harmonic interatomic force constants (IFCs)~~

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

- Will be supplied as supplemental material upon publication

* ~~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***

* ~~Four converged T-dependent thermal conductivities (~~*~~k~~*~~): natural isotopes with full BTE solution (~~*~~k~~~~nat,full~~*~~), natural isotopes with the relaxation time approximation (RTA) (~~*~~k~~~~nat,RTA~~*~~), isotopically pure (100%~~ ~~70~~~~Ge (69.924 amu)) with full BTE solution (~~*~~k~~~~pure,full~~*~~), and isotopically pure with RTA (~~*~~k~~~~pure,RTA~~*~~). If only RTA available, then only~~ *~~k~~~~nat,RTA~~* ~~and~~ *~~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 10K < T < 1000K (excel or text file)

- For 10K ≤ T ≤ 50K increments of 10K (5 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 10K to 1000K list (22 rows): T, *knat,full*, *knat,RTA*, *kpure,full*, *kpure,RTA*

* ~~Accumulated T=300K~~ *~~k~~~~acc~~* ~~vs frequency and~~ *~~k~~~~acc~~* ~~vs mean free path (mfp) for converged~~ *~~k~~~~nat,RTA~~* ~~value~~

- Numerical data for each mode (q, *j*) sampled in the Brillouin zone integration: f (THz), mfp=|sqrt(*vx*2+*vy*2+*vz*2)×lifetime| (nm), mode contribution to *k* (W/m/K) for *knat,RTA*

- 1 file (excel or text) with row for each mode (q, *j*): f, mfp, mode contribution to *k*

* ~~RTA T=300K three-phonon scattering rates (1/~~*~~τ~~~~3ph~~*~~) and phonon-isotope scattering rates for natural abundance (1/~~*~~τ~~~~iso~~*~~)~~

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

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

* ~~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=300K~~

- Varying integration meshes

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