MATERIALS CATALOG

Downloadable from our online database:

www.almabte.eu

FIRST-PRINCIPLES ATOMISTIC PROPERTIES

- crystal structure — POSCAR
- _metadata
- dielectric params. *polar compounds only* — BORN
- 2nd order, 3rd order — FORCE_CONSTANTS

Compound description <xml/>

VCAbuilder • superlattice_builder

single crystal | alloy | superlattice

Each compound needs to be built only once.

WAVEVECTOR-RESOLVED PHONON INFORMATION

Si .h5 | GaAs .h5 | $Si_{0.4}Ge_{0.6}$ .h5 | $Al_{0.1}Ga_{0.9}N$ .h5 | ... | $(A_{x\,nm}B_{y\,nm})_N$ .h5

THERMAL PROPERTY EXPLORERS

Computation settings <xml/>

Reference temperature

phononinfo

→ wavevectors, frequencies, lifetimes AT REF. TEMP., group velocities

kappa_Tsweep

RTA + full BTE

→ conductivity tensor, heat capacity VERSUS TEMPERATURE

kappa_crossplanefilms, kappa_inplanefilms

→ effective conductivity VERSUS FILM THICKNESS

cumulativecurves

→ cumul. conductivity, cumul. heat capacity RESOLVED BY PHONON METRICS

BTE SOLVERS

transient_analytic1d

→ single pulse response

steady_montecarlo1d

T_{hot} … T_{cold}

→ temperature profile, effective conductivity, spectral heat flux

steady_montecarlo1d_powersource

source … sink

→ temperature profile, effective conductivity, spectral heat flux

bte ALMA

Release 1.3

Operational Blueprint

Input provided by ALMA developers and/or external software

Software executable

Computation output saved to disc

User-generated input file

Command-line parameter