The basis.in input file

From GPUMD
Jump to navigationJump to search

Purpose

This file is used to define the unit cell for phonon calculations.

File format

- The format of this file must be as follows:

```
N_basis
id(0) mass(0)
id(1) mass(1)
...
id(N_basis-1) mass(N_basis-1)
map(0)
map(1)
...
map(N-1)
```

- Here,
  - `N_basis` is the number of atoms in the unit cell you choose. For example, it can be 2 for diamond silicon if you use the primitive cell as the unit cell.
  - The next `N_basis` lines contain the atom indices (using the order as in the xyz.in file; starting from 0) and masses for the basis atoms. For the example of diamond silicon, `id(0)=0` and `mass(0)=28` are the index and mass for the first basis atom, and `id(1)=4` and `mass(1)=28` are the index and mass for the second basis atom.
  - The remaining `N` lines map the `N` atoms in the xyz.in file to the basis atoms. If the `n`-th atom in the xyz.in file is equivalent to (under translation) the `m`-th basis atom in the unit cell, we have `map(n)=m`. In our example, `map(n)` is either 0 (equivalent to the first basis atom) or 1 (equivalent to the second basis atom).

Related pages

- See the tutorial on phonon dispersion for an explicit example.
