

The omega2.out output file

From GPUMD

[Jump to navigation](#)[Jump to search](#)

Purpose

This file contains the frequency square $\omega^2(\vec{k})$ at different k points.

File format

- It has `N_kpoints` rows and `3 * N_basis` columns, where `N_basis` is the number of basis atoms in the unit cell defined in the `basis.in` file and `N_kpoints` is the number of k points in the `kpoints.in` file.
- Each line corresponds to one k point. Each line has `3 * N_basis` numbers, corresponding to

the `3 * N_basis` values for $\omega^2(\vec{k})$ (in units of [THz]²) in the order of increasing magnitude.

Retrieved from "https://gpumd.zheyongfan.org/index.php?title=The_omega2.out_output_file&oldid=21391"

-
- This page was last edited on 23 August 2020, at 10:39.