The compute dos keyword

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Introduction

- This keyword computes the phonon density of states (PDOS) using the mass-weighted velocity autocorrelation (VAC). The output is normalized such that the integral of the PDOS over all frequencies equals $3N$, where N is the number of atoms. If this keyword appears in a run, the mass-weighted VAC will be computed and directly used to compute the PDOS.

Grammar

- For this keyword, the command looks like:

```
compute_dos sample_interval Nc omega_max <optional_args>
```

with parameters defined as:

- `sample_interval`: Sampling interval of the velocity data
- `Nc`: Maximum number of correlation steps
- `omega_max`: Maximum angular frequency $\omega_{max} = 2\pi\nu_{max}$ used in the PDOS calculations.

The `optional_args` provide additional functionality by allowing special keywords. The keywords for this function are `group` and `num_dos_points`. These keywords can be used in any order, but the parameters associated with each must follow exactly. The parameters are:

- `group group_method group`

    `group_method`: The grouping method to use for computation
    `group`: The group in the grouping method to use

- `num_dos_points points`

    `points`: Number of frequency points to be used in the DOS calculation (`Nc` if option not selected).

Examples

Example 1

- An example of this keyword is:

```
compute_dos 5 200 400.0 group 1 1 num_dos_points 300
```

This means that you (1) want to calculate the PDOS; (2) the velocity data will be recorded every 5 steps; (3) the maximum number of correlation steps is 200; (4) the maximum angular frequency you want to consider is $\omega_{max} = 2\pi\nu_{max} = 400$ THz; (5) You would like to compute only over group 1 in group method 1; (5) You would like the maximum angular frequency to be cut in to 300 points for output. The results will be written into files named mvac.out for the mass-normalized VAC and dos.out for the DOS output.

Caveats

- Cannot be used in the same run as the compute_sdc keyword.

Output files

- dos.out
- mvac.out

Related tutorial

- Tutorial: Density of states

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