

The delta keyword

From GPUMD

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Purpose

- This keyword is used to specify a displacement for calculating the force constants using the finite-displacement method.

Grammar

- It only has one parameter, which is the displacement (in units of Å) for calculating the force constants.

Examples

- To set a displacement of 0.005 Å, just write

```
delta 0.005
```

Tips

- We recommend a value between 0.001 Å and 0.01 Å for the displacement.

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