The cutoff keyword

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Purpose

- This keyword is used to specify a cutoff distance for calculating the force constants.

Grammar

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

Examples

- To set a cutoff distance of 4 A, just write

```
cutoff 4
```

Tips

- For two-body potentials, the cutoff distance for force constants can be the same as that for force evaluations. However, for many-body potentials, the cutoff distance for force constants should be larger than that for force evaluations. Consider diamond silicon described by the Tersoff potential, one only needs to consider first-nearest neighbors for force evaluation, but one has to also consider second-nearest neighbors for force constant calculations.

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