The Lennard-Jones potential

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Brief descriptions

- This is the Lennard-Jones (LJ) potential.
- It applies to systems with up to 10 atom types.
- The potential has not been shifted or damped.

Potential form

- The LJ potential is one of the most simplest two-body potentials used in MD simulations. The pair potential between particles i and j is

$$U_{ij} = 4\epsilon_{ij} \left(\frac{\sigma_{ij}^{12}}{r_{ij}^{12}} - \frac{\sigma_{ij}^{6}}{r_{ij}^{6}} \right).$$

Parameters

Parameter	Units
ϵ_{ij}	eV
σ_{ij}	A

Potential file format

- If there is only one atom type, the potential file for this potential model reads

```
lj 1
epsilon sigma cutoff
```

Here, `cutoff` is the cutoff distance.

- If there are two atom types, the potential file reads

```
lj 2
epsilon_00 sigma_00 cutoff_00
epsilon_01 sigma_01 cutoff_01
```

```
epsilon_10 sigma_10 cutoff_10
epsilon_11 sigma_11 cutoff_11
```

- If there are three atom types, the potential file reads

```
lj 3
epsilon_00 sigma_00 cutoff_00
epsilon_01 sigma_01 cutoff_01
epsilon_02 sigma_02 cutoff_02
epsilon_10 sigma_10 cutoff_10
epsilon_11 sigma_11 cutoff_11
epsilon_12 sigma_12 cutoff_12
epsilon_20 sigma_20 cutoff_20
epsilon_21 sigma_21 cutoff_21
epsilon_22 sigma_22 cutoff_22
```

- I hope the reader can understand the pattern and figure out how to prepare potential files with more atom types.

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