Lennard-Jones Potential

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1 Lennard-Jones Potential

A Lennard-Jones (LJ) potential $V(r_{ij})$ between two atoms placed at distance $r_{ij} = |\mathbf{r}_j - \mathbf{r}_i|$ is defined by:

$$V(r_{ij}) = 4\epsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right]. \tag{1}$$

And the force on atom i produced by LJ potetial is

$$\mathbf{F}_i = -\frac{24\epsilon}{r_{ij}} \left[2 \left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right] \hat{\mathbf{r}}_{ij}, \tag{2}$$

where

$$\hat{\mathbf{r}}_{ij} = \frac{\mathbf{r}_{ij}}{r_{ij}} = \frac{x_{ij}\hat{\mathbf{x}} + y_{ij}\hat{\mathbf{y}} + z_{ij}\hat{\mathbf{z}}}{\sqrt{x_{ij}^2 + y_{ij}^2 + z_{ij}^2}}. \tag{3}$$

Similarly, the force on atom j is

$$\mathbf{F}_j = \frac{24\epsilon}{r_{ij}} \left[2 \left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right] \hat{\mathbf{r}}_{ij}, \tag{4}$$

which is just opposite to $\mathbf{F}_i$.