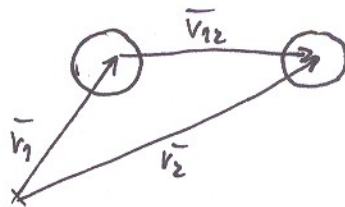


## L-J potenciál

$$U_{LJ} = 4\epsilon \left[ \left( \frac{\sigma}{r_{12}} \right)^{12} - \left( \frac{\sigma}{r_{12}} \right)^6 \right]$$



$$\vec{r}_1 = x_1 \vec{a} + y_1 \vec{b}$$

$$\vec{r}_2 = x_2 \vec{a} + y_2 \vec{b}$$

$$\vec{r}_{12} = \vec{r}_2 - \vec{r}_1$$

$$\vec{r}_{12} = x_{12} \vec{a} + y_{12} \vec{b}$$

$$F = -\frac{\partial U}{\partial r_{12}} = 4\epsilon \frac{1}{r_{12}} \left[ 12 \left( \frac{\sigma}{r_{12}} \right)^{12} - 6 \left( \frac{\sigma}{r_{12}} \right)^6 \right]$$

$$F_{1x} = 4\epsilon \frac{1}{r_{12}} \left[ 12 \left( \frac{\sigma}{r_{12}} \right)^{12} - 6 \left( \frac{\sigma}{r_{12}} \right)^6 \right] \frac{x_{12}}{r_{12}} \quad F_{1y} = 4\epsilon \frac{1}{r_{12}} \left[ 12 \left( \frac{\sigma}{r_{12}} \right)^{12} - 6 \left( \frac{\sigma}{r_{12}} \right)^6 \right] \frac{y_{12}}{r_{12}}$$

$$F_{2x} = -F_{1x}$$

$$F_{2y} = -F_{1y}$$

$$R_{\text{cutoff}} \geq 3\sigma$$

$$\text{MIC: } \frac{B}{Z} \geq R_{\text{cutoff}}$$

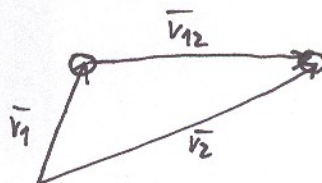
pln	$E/k_B [K]$	$\sigma [\text{nm}]$
H	8,6	0,287
He	10,2	0,228
C	57,2	0,335
N	37,3	0,337
O	67,6	0,296
Ar	120	0,37

## Coulombický potenciál

$$\vec{F}_c = \frac{1}{4\pi\epsilon_0} \frac{q_1 q_2}{r_{12}^3} \vec{r}_{12} = \frac{A}{r_{12}^3} \vec{r}_{12}$$

$$\vec{F}_1 = -\vec{F}_c$$

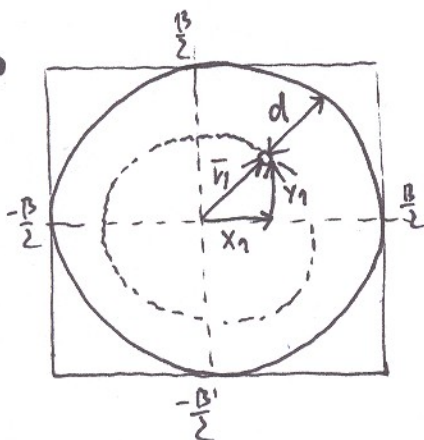
$$\vec{F}_2 = \vec{F}_c$$



$$\vec{r}_{12} = \vec{r}_2 - \vec{r}_1$$

$$A = 8,987$$

$$W = 1,0$$



$$\vec{F}_s = -\frac{A}{d^2} \frac{\vec{r}_1}{|\vec{r}_1|}$$

$$\vec{F}_v = -k\vec{r}$$