

1. Bond potential

$$V(x) = \frac{1}{2}k(x - x_{\text{eq}})^2$$

$$V(x) = D_e \left(1 - e^{-a(x-x_{\text{eq}})}\right)^2$$

$$V(x) = k_{\text{ub}}(x - x_{\text{eq}})^2$$

$$V(x) = K(x^2 - x_0^2)^2$$

$$V(x) = \frac{\phi(x - x_0)^2}{[\lambda^2 - (x - x_0)^2]}$$

2. Angle potential

$$V(x) = k(x - x_{\text{eq}})^2$$

$$V(x) = k_{\theta} \sin^2 \left(\frac{nx}{2} \right)$$

$$V(x) = \frac{1}{2}k_{\theta} (\cos(x) - \cos(x_{\text{eq}}))^2$$

$$V(x) = K [1 + \cos(x)]$$

$$V(x) = \frac{2.0}{n^2} \cdot C [1 - B(-1)^n \cos(nx)]$$

$$V(x) = K_2(x - x_0)^2 + K_3(x - x_0)^3 + K_4(x - x_0)^4$$

3. Dihedral potential

$$V(x) = k(x - x_{\text{eq}})^2$$

$$V(x) = k [1 + \cos(nx - \delta)]$$

$$V(x) = V_1 (1 + \cos(x)) + V_2 (1 - \cos(2x)) + V_3 (1 + \cos(3x)) + V_4 (1 - \cos(4x))$$

$$V(x) = V_1 (1 + \cos(x)) + V_2 (1 - \cos(2x))$$

$$V(x) = V_1 (1 + \cos(x))$$

$$V(x) = \frac{1}{2}V_0 (1 + \cos(x))$$

$$V(x) = V_0 (1 + \cos(nx))$$

$$V(x) = V_0 \left(1 - e^{-\alpha(x-x_0)^2}\right)$$

$$V(x) = V_0 \left(1 - e^{-\alpha(\cos(x) - \cos(x_0))^2}\right)$$

$$V(x) = V_0 \left(1 - e^{-\alpha(\sin(x))^2}\right)$$

$$V(x) = A [1 - \cos(x)] + B [1 + \cos(3x)] + C \left[1 + \cos\left(x + \frac{\pi}{4}\right)\right]$$

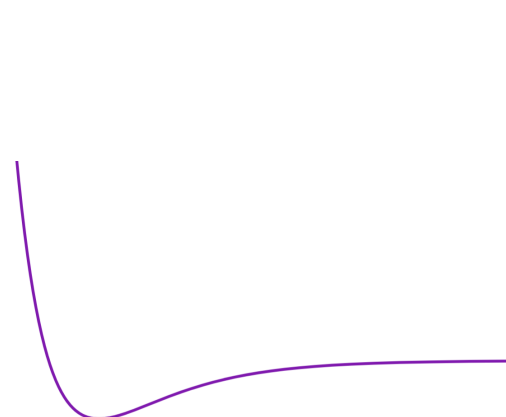
$$V(x) = \sum_{n=1,5} A_n \cos^{n-1}(x)$$

4. van der Waals potential (non-bonded)

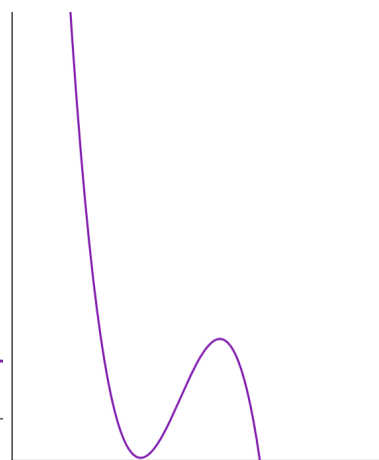
$$V_{NB}(x) = Ae^{-(x/\rho)} - \frac{C}{x^6}$$

$$V_{NB}(x) = \epsilon \left(\left[\frac{\sigma}{x} \right]^9 - 3 \left[\frac{\sigma}{x} \right]^6 \right)$$

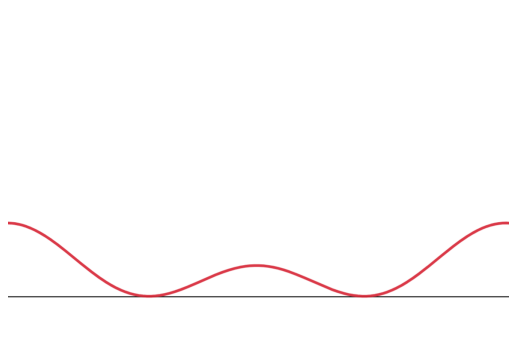
$$V_{NB}(x) = 4\epsilon \left(\left[\frac{\sigma}{x} \right]^{12} - \left[\frac{\sigma}{x} \right]^6 \right)$$



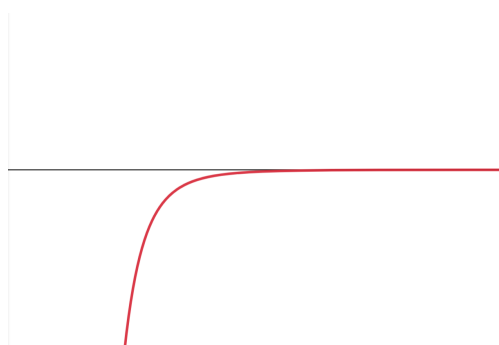
(a) Bond Potential



(b) Angle Potential



(c) Dihedral Potential



(d) van der Waals Potential