Biophysics of Macromolecules SS 2020

PROBLEM SET 1

① a) Volume of E. coli:

$$V = \pi R^2 \cdot L = \pi \left(\tfrac{1}{2} 10^{-6}\,m\right)^2 \cdot 2 \cdot 10^{-6}\,m$$

$$= 1.6 \cdot 10^{-18}\,m^3 \approx 1\,\mu m^3$$

$$\approx 1\,fl$$

b) $1\,nM \Rightarrow \dfrac{10^{-9} \cdot 6 \cdot 10^{23}\ \text{molecules}}{1\,l}$

$$= \frac{0.6\ \text{molecules}}{1\,fl}$$

$\Rightarrow$ Roughly 1 molecule per E. coli cell.

$1\,mM \Rightarrow \dfrac{10^{-3} \cdot 6 \cdot 10^{23}\ \text{molecules}}{1\,l}$

$$= \frac{600\,000\ \text{molecules}}{1\,fl}$$

$\rightarrow$ Roughly 10^6 molecules per E. coli.

$1\,M \Rightarrow \dfrac{6 \cdot 10^{23}\ \text{molecules}}{1\,l} = \dfrac{6 \cdot 10^{8}\ \text{molec.}}{1\,fl}$

$\Rightarrow$ Roughly 10^9 molecules per E. coli.

c) Spacing on cubic lattice: $d = c^{-1/3}$

$$1\,nM \Rightarrow d = \left(\frac{10^{-9} \cdot 6 \cdot 10^{23}}{10^{-3}\,m^3}\right)^{-1/3}$$

$$\approx 10^{-6}\,m = \underline{\underline{1\,\mu m}}$$

$$1\,mM \Rightarrow d = \left(\frac{10^{-3} \cdot 6 \cdot 10^{23}}{10^{-3}\,m^3}\right)^{-1/3}$$

$$\approx \underline{\underline{10\,nm}}$$

$$1\,M \Rightarrow d = \left(\frac{6 \cdot 10^{23}}{10^{-3}\,m^3}\right)^{-1/3} \approx \underline{\underline{1\,nm}}$$

d) Mass of E. coli, assuming $\rho_{H_2O} = 1000\,\frac{kg}{m^3}$

$$\Rightarrow m_{E.coli} = \rho_{H_2O} \cdot V_{E.coli} = 10^3\,\frac{kg}{m^3} \cdot 10^{-18}\,m^3$$

$$= 10^{-15}\,kg = \underline{\underline{1\,pg}}$$

e) E. coli is slightly denser than water; $\rho_{E.coli} \approx 1100\,kg/m^3$, due to protein & nucleic acid content. One consequence is that you can sediment E. coli by centrifugation.

k) $30\,\mu m/s$ corresponds to $\sim 15 \frac{\text{body length}}{s}$

- World class human swimmers swim the 100 m freestyle in < 1 min (the current world record is just under 47s);

$$\Rightarrow V_{human} = \frac{100\,m}{47\,s} \approx 2\,\frac{m}{s} \approx \frac{1\text{ body length}}{s};$$

- Great white sharks are ≈ 5 m long and swim up to 30 mph $\approx 13\,m/s$

$$\Rightarrow V_{shark} = 13\,m/s \approx 2.5\,\frac{\text{body length}}{s}$$

So E. coli outswim both humans and sharks, normalized to body size.

(2) Energy release in ATP hydrolysis.

$$U(r)_{\text{Coulomb}} = \frac{1}{4\pi\varepsilon\varepsilon_0}\frac{q_1 q_2}{r_{12}} \quad \text{in general}$$

i.e. the Coulomb energy of two charges q_1 & q_2 at a distance r_{12}.

Energy change in hydrolysis: $\Delta E = E_{ATP} - E_{ADP}$

$$E_{ATP} = \frac{1}{4\pi\varepsilon\varepsilon_0}\left(\underbrace{\frac{e^2}{0.3\,\text{nm}}}_{\substack{\alpha \text{ to } \beta\\ \text{phosphate}}} + \underbrace{\frac{2e^2}{0.3\,\text{nm}}}_{\substack{\beta \text{ to } \gamma\\ \text{phosphate}}} + \underbrace{\frac{2e^2}{0.6\,\text{nm}}}_{\substack{\alpha \text{ to } \gamma\\ \text{phosphate}}}\right)$$

$$E_{ADP} = \frac{1}{4\pi\varepsilon\varepsilon_0}\frac{e^2}{0.3\,\text{nm}}$$

$$\Delta E = \frac{1}{4\pi\varepsilon\varepsilon_0}\left(\frac{2e^2}{0.3\,\text{nm}} + \frac{2e^2}{0.6\,\text{nm}}\right)$$

$$= \frac{1}{4\pi\varepsilon\varepsilon_0}\cdot\frac{e^2}{0.1\,\text{nm}}$$

For $\varepsilon = 1$: $\Delta E = \dfrac{1}{4\pi\cdot 8.85\cdot 10^{-12}\,\frac{C^2}{N^2 m^2}}\,\dfrac{(1.6\cdot 10^{-19}\,C)^2}{0.1\cdot 10^{-9}\,m}$

$$= 2.3\cdot 10^{-18}\,\text{N}\cdot\text{m} \approx 330\,\frac{\text{kcal}}{\text{mol}} \approx 560\,k_BT$$

In water $\varepsilon \cong 80$

For $\varepsilon = 80 \Rightarrow \Delta E = \dfrac{560\,k_BT}{80} \approx 7\,k_BT$

(3) van der Waals interaction with repulsive term:

$$E(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

a) Minimum of the energy at $r = r^*$

$$\frac{dE}{dr} \overset{!}{=} 0 = 4\varepsilon\left(-12\frac{\sigma^{12}}{r^{13}} + 6\frac{\sigma^6}{r^7}\right)$$

$$\Rightarrow 12\frac{\sigma^{12}}{r^{13}} = 6\frac{\sigma^6}{r^7}$$

$$\Rightarrow 2\sigma^6 = r^6$$

$\Rightarrow$ Minimum at $r^* = 2^{1/6}\sigma \cong 1.12\,\sigma$

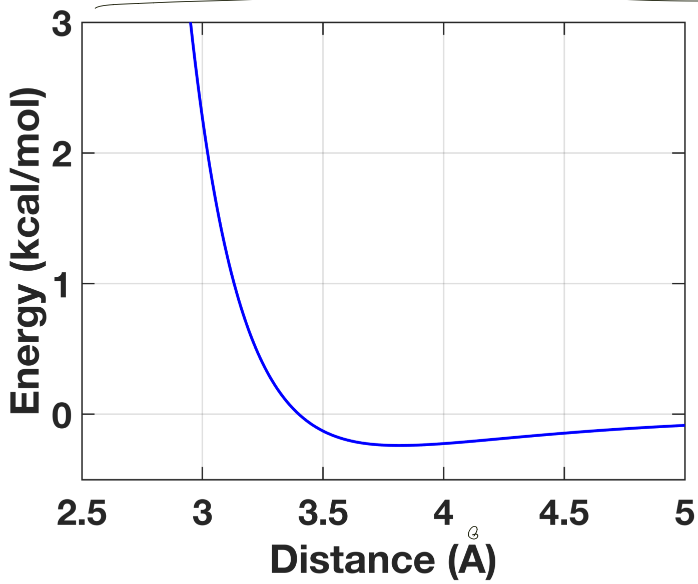
Energy at minimum:

$$E(r^*) = 4\varepsilon\left(\frac{\sigma^{12}}{2^{12/6}\sigma^{12}} - \frac{\sigma^6}{2^{6/6}\sigma^6}\right)$$

$$= 4\varepsilon\left(\frac{1}{4} - \frac{1}{2}\right) = \underline{\underline{-\varepsilon}}$$

b) Plot of the function
(see matlab code for details):

Lennard-Jones potential:



c) Interpretation of the terms:

- The $\frac{1}{r^6}$ - term is attractive and due to induced dipole - induced dipole dispersion forces, at intermediate distances. The $1/r^6$ dependence can be derived from 2^{nd} order perturbation theory.
- The $1/r^{12}$ - term is repulsive at short distances; it keeps atoms from overlapping and can be thought of as a manifestation of the Pauli exclusion principle. Sometimes it is also parametrized as $\sim 1/r^{12}$.