Biophysics of Macromolecules SS 2021

PROBLEM SET 1

① a) Volume of E. coli:

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

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

$$\approx 1 fl$$

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

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

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

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

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

$\Rightarrow$ Roughly 106 molecules per E. coli.

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

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

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

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

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

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

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

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

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

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

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

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

k) 30 μm/s corresponds to ~15 $\frac{\text{body length}}{\text{s}}$

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

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

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

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

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

② Energy release in ATP hydrolysis.

$U(r)_{\text{Coulomb}} = \frac{1}{4\pi\varepsilon\varepsilon_0}\frac{q_1 q_2}{r_{1,2}}$ in general

i.e. the Coulomb energy of two charges q_1 & q_2 at a distance $r_{1,2}$.

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

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

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

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

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

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

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

$\approx 560\,k_B T$

In water $\varepsilon \cong 80$

For $\varepsilon = 80 \Rightarrow \Delta E = \frac{560\,k_B T}{80} \approx 7\,k_B T$

(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 $r = r^*$

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

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

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

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

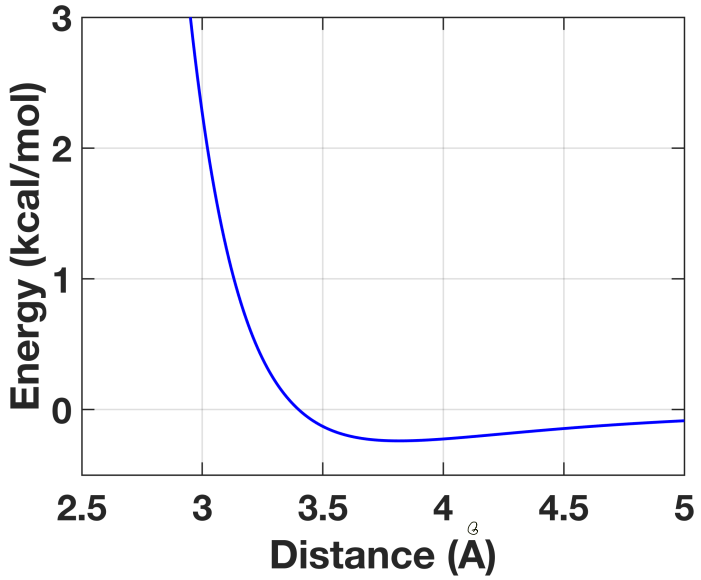
Energy at minimum:

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

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

b) Plot of the function

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 2nd 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 $\sim 1/r^{12}$.