

25/75%

NORWEGIAN UNIVERSITY OF SCIENCE AND TECHNOLOGY  
Department of Physics

Contacts during the exam:  
*Pawel Sikorski*, phone: 98486426

## EXAM TFY4335 BIONANOTECHNOLOGY

Monday 18th of May 2009. 09:00

### Examination support materials:

- Formula sheet - see Appendix A
- Simple calculator (according to NTNU exam regulations)
- K. Rottmann: Matematisk formelsamling (eller tilsvarende)
- Carl Angell og Bjørn Ebbe Lian: Fysiske størrelser og enheter, navn og symboler (eller tilsvarende)

Answer must be written in English or Norwegian. Exam consists of five (5) main questions with sub-questions. Number of points given to each sub-question is given in bold font. The maximum score for the exam is **75p**.

### Question 1: Short questions (15p)

1. Define bionanotechnology(**3p**)
2. How big are (choose the closest answer):
  - white blood cell:  $0.1\mu m$ ,  $1\mu m$ ,  $10\mu m$ ,  $100\mu m$  (**1p**)
  - bacteria (e.coli):  $0.1\mu m$ ,  $1\mu m$ ,  $10\mu m$ ,  $100\mu m$ ; (**1p**)
  - diameter (width) of DNA double helix:  $0.2nm$ ,  $2nm$ ,  $5nm$ ,  $15nm$ ,  $25nm$  (**1p**)
3. What is  $x_0$  defined by:

$$x_0 = \left( \frac{e}{2\pi\epsilon_B\sigma_q} \right)$$

(**3p**)

4. What is usually described by Freely Joint Chain model (FJC) (**2p**)
5. What are capillary driven microfluidic devices and how are they different from general microfluidic devices (**2p**)
6. What is Elastin.(**3p**)

**Question 2 Interactions (20p)**

1. What are the interaction holding folded protein molecules together. List and comment on length-scales (distances) at which interacting parts of the molecules starts to feel an attractive/repulsive force. (5p)
2. Figure 9 shows formation of a complex **AB** between molecule **A** and **B**. Explain why shapes of both molecules and chemical properties of both surfaces involved in the interactions are important. Explain, how nature is able to design matching molecular pairs, which bind very strongly to each other, but not to any other molecule inside a cell. Appendix B list chemical structure of amino acids involved in the interactions for those two proteins (marked on the Figure 9). (5p)

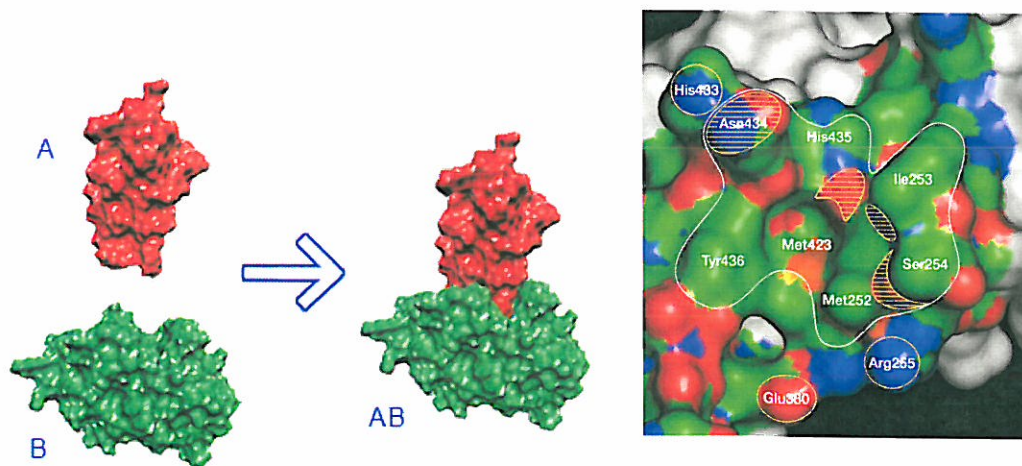
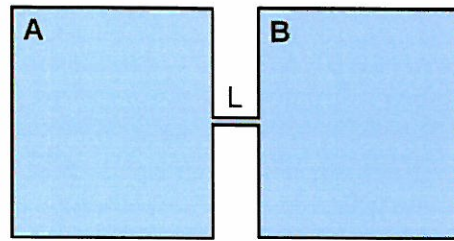


Figure 1: Binding between two protein molecules. Although protein-protein interactions occur over a large surface area, X-ray crystallography have shown that many protein-protein interfaces contain compact, centralized regions of residues - 'hot spots' - that are crucial for the interaction. The binding site is colored by atom type and the consensus binding site is outlined.

3. Denaturation is a process of "forced" unfolding of a protein molecule. Which of the following environmental changes is likely to enhance denaturation. Shortly explain why.
  - raising the temperature (2p)
  - replacing surrounding water with non-polar solvent (2p)
  - increasing amount of salt in solution (2p)
4. What is defined by **depletion force** and how this force is important for interaction between large protein molecules inside a cell. (4p)

**Question 3 Transport (20p)**

1. Equation 13 (diffusion equation in 1D, Appendix A) describes how local concentration of dissolved molecules will change with time due to diffusion. Imagine two large containers connected through a narrow channel with a circular cross-section (radius: 100  $\mu\text{m}$ , length  $L = 1\text{ cm}$ ) as shown in Figure 10.  
 Container **A** contains 0.02M solution of Glucose and 0.01M solution of Ethanol in water.  
 Container **B** contains 0.02M solution of Ethanol in water.



Figur 2: Experimental setup

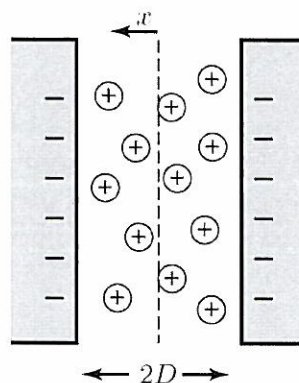
- What will be a **steady state** situation for the system shown above. Solve diffusion equation for a steady state situation, calculate and plot concentration profiles for Glucose and Ethanol inside the channel. (10p)
  - Will the concentration profile of Glucose inside the channel depend on the concentration of Ethanol inside the channel? (1p)
  - Will the flux of Glucose molecules depend on the flux of Ethanol molecules. (1p)
  - How will the concentration profiles and flux  $j$  through the channel depend on the channel width? (3p)
2. What is defined by Reynolds number? What range of Reynolds number typically describe nano- and micro-fluidics devices. Calculate Reynolds number for a microfluidic device with a channel width of  $1 \times 10^{-6} \text{ m}$  and fluid velocity of  $1 \times 10^{-6} \text{ ms}^{-1}$ ). What consequences do this Reynolds number has to the properties of water at those length scales. (5p)

#### Question 4 Entropic forces (10p)

At macro-scale, mechanical force is defined as a change in potential energy  $U$  with respect to some state variable  $x$ :

$$f = -\frac{dU}{dx}$$

- defined entropic force and list some examples; (4p)
- which of those forces will be important for a living cell, explain how; (3p)
- What is a origin of repulsion force between two charged surfaces shown in Figure 11 when they are placed in water containing some dissolved NaCl. How would the situation be different in vacuum (no water and no salt). (3p)



Figur 3: Repulsion between two charged surfaces

**Question 5 Molecular Motors (10p)**

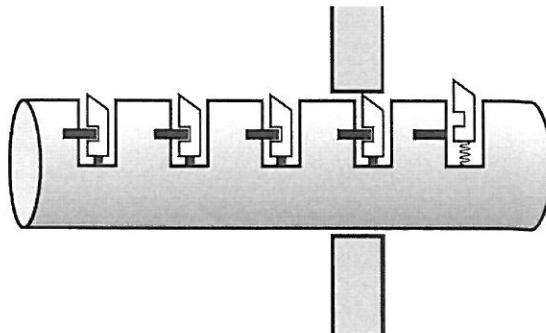
Why is diffusion important in describing the behavior of molecular motors. Equation 64 (Appendix A) describes the velocity of idealized molecular motor based on S-ratchet concept (Fig 12).

1. Show that in a absence of external load, the motor speed will be:

$$v = \frac{2D}{L}$$

Hint: use  $e^{\bar{f}} = 1 + \bar{f} + \frac{1}{2}\bar{f}^2$ , with  $\bar{f} = \frac{fL}{k_B T}$  (3p)

2. Calculate  $v$  for a motor making steps of 9nm. This motor is a protein molecule with a spherical shape and diameter of 20nm. (3p)
3. For a real molecular motor, what other factors will affect the speed at which it is moving. What is a typical source of energy for molecular motors found in cells and when they move a long the track pulling a load, what is this energy used for. (4p)



Figur 4: S-ratchet

NORWEGIAN UNIVERSITY OF SCIENCE AND TECHNOLOGY  
Department of Physics

Contacts during the exam:  
*Pawel Sikorski*, phone: 98486426

## EKSAMEN TFY4335 BIONANOTECHNOLOGY

Mandag 18th of Mai 2009. 09:00

### Tillatte hjelpemidler under eksamen:

- formelark: se appendiks A
- enkel kalkulator (i henhold til NTNUs eksamensregulativ)
- K. Rottmann: Matematisk formelsamling (eller tilsvarende)
- Carl Angell og Bjørn Ebbe Lian: Fysiske størrelser og enheter, navn og symboler (eller tilsvarende)

Besvarelsen kan skrives på engelsk eller norsk. Eksamen består av fem (5) oppgaver, hver med delspørsmål. Poeng for hvert delspørsmål er angitt. Maksimal poengsum for eksamen er **75p**.

### Oppgave 1: Kortsvars oppgave (15p)

1. Definer bionanoteknologi(**3p**)
2. hvor stor er (velg alternativet som ligger nærmest):
  - en hvit blodcelle:  $0.1\mu m$ ,  $1\mu m$ ,  $10\mu m$ ,  $100\mu m$  (**1p**)
  - bakterie (e. coli):  $0.1\mu m$ ,  $1\mu m$ ,  $10\mu m$ ,  $100\mu m$  (**1p**)
  - diameter til DNA dobbel heliks:  $0.2nm$ ,  $2nm$ ,  $5nm$ ,  $15nm$ ,  $25nm$  (**1p**)
3.  $x_0$  er definert ved uttrykket under. Hva er  $x_0$ ? (**3p**)

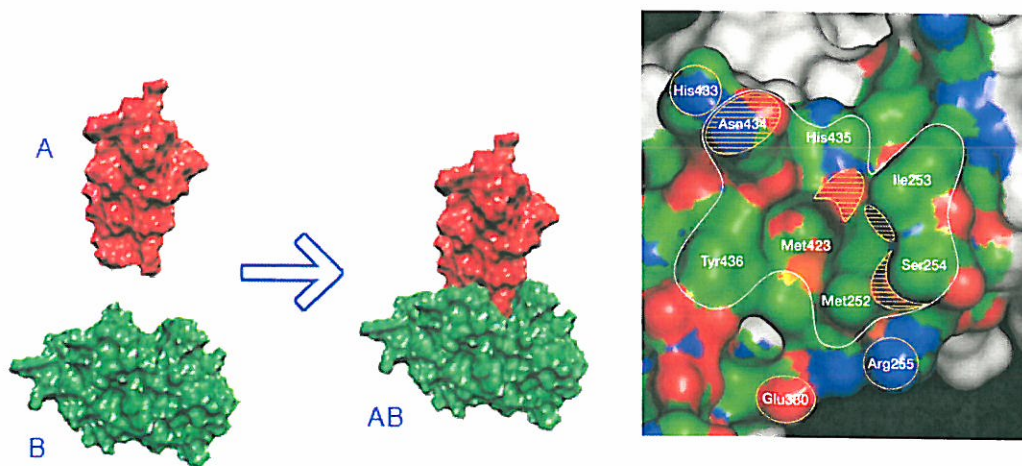
$$x_0 = \left( \frac{e}{2\pi\ell_B\sigma_q} \right)$$

4. Hva beskrives vanligvis ved "Freely Joint Chain" (FJC) modellen ? (**2p**)
5. Hva er kapillær drevne "microfluidic devices" og hvordan skiller de seg fra generelle "microfluidic devices"? (**2p**)
6. Hva er elastin?(**2p**)



### Oppgave 2: Vekselvirkninger (20p)

1. Hvilke vekselvirkninger holder foldede proteiner sammen? List opp og kommenter på hvilke lengdeskalaer (avstander) ulike vekselvirkende deler av molekylene begynner å føle en attraktiv/frastøtende kraft. (5p)
2. Figur 9 viser dannelsen av et kompleks AB mellom molekyl A og molekyl B. Forklar hvorfor formen til begge molekylene og de kjemiske egenskapene til begge overflatene involvert i vekselvirkningen er viktige. Forklar hvordan naturen er i stand til å designe matchende molekylpar som bindes veldig sterkt til hverandre men ikke til andre molekyler inne i en celle. Appendiks B viser kjemisk struktur til aminosyrer som er involvert i vekselvirkningen mellom de to proteinene som er vist i figur 9. (5p)

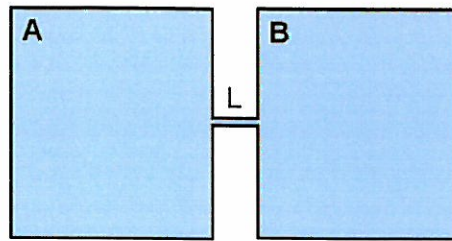


Figur 5: Binding mellom to protein molekyler. Selv om protein-protein vekselvirkninger foregår over et stort overflate areal har røntgen krystallografi vist at mange protein-protein grenseflater inneholder kompakte, sentraliserte områder av residuer – hot spots – som er avgjørende for vekselvirkningen. Bindingssete er farget etter atomtype.

3. Denaturering er en prosess som kan beskrives som tvunget “unfolding” av et proteinmolekyl. Hvilke av de følgende forandringene i miljøet vil sannsynligvis fremme denaturering. Forklar kort hvorfor.
  - økt temperatur (2p)
  - utskifting av vannet i omgivelsene med et ikke-polart løsningsmiddel (2p)
  - økt mengde salt i løsningen (2p)
4. Hva er definert med “depletion” kraft, og hvordan er denne kraften viktig for vekselvirkningen mellom store protein molekyler inne i en celle? (4p)

### Oppgave 3: Transport (20p)

1. Ligning 13 (diffusjonsligningen i 1D, appendiks A) beskriver hvordan den lokale konsentrasjonen av molekyler i løsning vil forandres som funksjon av tid på grunn av diffusjon. Se for deg to store beholdere som er forbundet gjennom en smal kanal med sirkulært tverrsnitt (radius  $100\ \mu\text{m}$ , lengde  $L = 1\ \text{cm}$ ), som vist i figur 10. Beholder A inneholder  $0.02\text{M}$  glukose og  $0.01\text{M}$  etanol i vann. Beholder B inneholder  $0.02\text{M}$  etanol i vann.



Figur 6: Forsøksoppsett

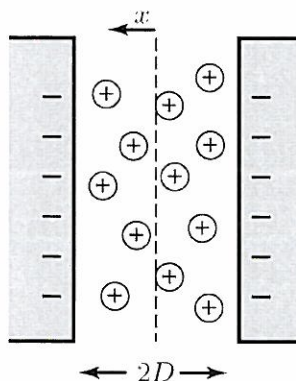
- Hva vil være stabil tilstand ("steady state") for dette systemet i figur 10? Los diffusjonsligningen for en "steady state" tilstand, beregn og tegn konsentrasjonsprofiler for glukose og etanol inne i kanalen. (10p)
  - vil konsentrasjonsprofilen av glukose i kanalen avhenge av konsentrasjonen av etanol inne i kanalen? (1p)
  - Vil fluksen av glukose molekyler avhenge av fluksen av etanol molekyler? (1p)
  - Hvordan vil konsentrasjonsprofilene og fluks  $j$  gjennom kanalen avhenge av diameteren på kanalen som forbinder de to beholderne? (3p)
2. Hva er definert av Reynolds nummer? Hvilket område av Reynolds nummer er typisk for nano- og mikrofluid "devices"? Beregn Reynolds nummer for et mikrofluid "devices" med kanalvidde på  $1 \times 10^{-6} \text{ m}$  og hastighet til løsningen på  $1 \times 10^{-6} \text{ ms}^{-1}$ . Hvilke konsekvenser har det Reynolds nummer for egenskapene til vann på disse lengdeskalaene? (5p)

#### Oppgave 4 Entropi krefter (Entropic forces) (10p)

På makronivå er mekanisk kraft definert som en forandring i potensiell energi  $U$  med hensyn på en tilstands variabel  $x$ .

$$f = -\frac{dU}{dx}$$

- definer entropi kraft og gi noen eksempler; (4p)
- hvilke av de kreftene vil være viktige for en levende celle, forklar hvorfor; (3p)
- Hva er opphavet til den frastøtende kraften mellom to ladete overflater, vist i figur 11, når de er plassert i vann som inneholder noe oppløst NaCl? Hvordan vil situasjonen være annerledes i vakuum (ikke noe vann eller salt)? (3p)



Figur 7: Frastøtning mellom to ladete overflater

**Oppgave 5: Molekylære motorer (10p)**

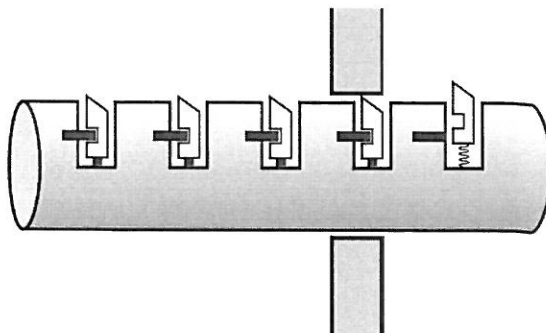
Hvorfor er diffusjon viktig for å beskrive oppførselen til molekylære motorer? Ligning 64 (appendiks A) beskriver hastigheten til en idealisert molekylær motor basert på "S-ratchet" konseptet (figur 12).

1. Vis at i fravær av en ekstern belastning blir hastigheten til motoren:

$$v = \frac{2D}{L}$$

Tips: bruk  $e^{\bar{f}} = 1 + \bar{f} + \frac{1}{2}\bar{f}^2$ , med  $\bar{f} = \frac{fL}{k_B T}$  (3p)

2. Beregn  $v$  for en skrittlengde på 9nm foretatt av en motor som er et sfærisk protein molekyl med en diameter på 20nm. (3p)
3. For en reell molekylær motor, hvilke andre faktorer vil påvirke hastigheten til motoren? Hva er typisk energi kilde for molekylære motorer som finnes i celler, og hva blir denne energien brukt til når de beveger seg langs sporet trekkende på en last? (4p)



Figur 8: "S-ratchet"



NORWEGIAN UNIVERSITY OF SCIENCE AND TECHNOLOGY  
Department of Physics

Contacts during the exam:  
*Pawel Sikorski*, phone: 98486426

## ANSWERS TO THE EXAM TFY4335 BIONANOTECHNOLOGY

Monday 18th of May 2009. 09:00

### Examination support materials:

- Formula sheet - see Appendix A
- Simple calculator (according to NTNU exam regulations)
- K. Rottmann: Matematisk formelsamling (eller tilsvarende)
- Carl Angell og Bjørn Ebbe Lian: Fysiske størrelser og enheter, navn og symboler (eller tilsvarende)

Answer must be written in English or Norwegian. Exam consists of five (5) main questions with sub-questions. Number of points given to each sub-question is given in bold font. The maximum score for the exam is **75p**.

### Question 1: Short questions (15p)

1. Define bionanotechnology(**3p**)

branch of nanotechnology which has medical applications, uses biological materials or biological design principles

2. How big are (choose the closest answer):

- white blood cell:  $0.1\mu m$ ,  $1\mu m$ ,  $10\mu m$ ,  $100\mu m$  (**1p**)
- bacteria (e.coli):  $0.1\mu m$ ,  $1\mu m$ ,  $10\mu m$ ,  $100\mu m$ ; (**1p**)
- diameter (width) of DNA double helix:  $0.2nm$ ,  $2nm$ ,  $5nm$ ,  $15nm$ ,  $25nm$  (**1p**)

3. What is  $x_0$  defined by:

$$x_0 = \left( \frac{e}{2\pi\ell_B\sigma_q} \right)$$

(**3p**)

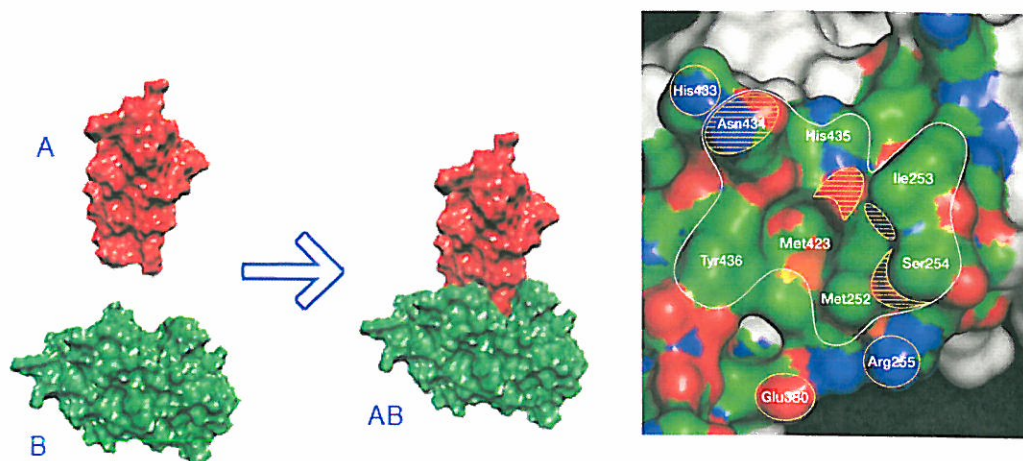
This is so called Gouy-Chapman length describing the thickness of diffuse charge layer close to a surface with a charge density  $\sigma_q$  in pure water (just enough ions in the solution to make the system neutral. absence of salt)

4. What is usually described by Freely Joint Chain model (FJC) (2p)  
 simplest possible model do describe mechanical properties (force-extension behavior) of a single polymer chain. In this approach polymer chain is approximated as a series of straight stiff segments connected by fully flexible joints. Model has one variable parameter - segment length. This segment length is generally not connected to chemical repeat - length of the monomer unit.
5. What are capillary driven microfluidic devices and how are they different from general microfluidic devices (2p)  
 in those devices liquid is pumped by a capillary pump - device contains large porous array which will be filled with the liquid by capillary force, driving at the same time the liquid into the device. Normal microfluidics devices use for example mechanical pumps.
6. What is Elastin.(3p)  
 Elastin is a protein from which parts of the human body which need rubber-like mechanical properties are made.

## Question 2 Interactions (20p)

1. What are the interaction holding folded protein molecules together. List and comment on length-scales (distances) at which interacting parts of the molecules starts to feel an attractive/repulsive force. (5p)
  - hydrogen bonding. energy gain from forming single hydrogen bond between two parts of a protein molecule is  $1-2 k_B T$ , there is also entropic contribution, as protein molecule forms h-bonds with itself it does not need to involve solvent water molecules. hydrogen bonding to water reduces entropy of water molecules. Short range - c.a. size of few water molecule
  - interactions between charge aa. short range due to screening in solution. Only important if aa are closer then  $\lambda_D$  which is 0.3nm for 1M NaCl and 1nm for 0.1 M NaCl solutions.
  - hydrophobic interactions. Originate in increase of entropy of water molecules if two hydrophobic groups stick together. In case where they are separated, water molecules form cage-like structures around hydrophobic groups. In this way water molecules can still make maximum number of h-bonds with each other, but sacrifice entropy. Hydrophobic interactions get stronger with increased temperature. Also short range - c.a. size of few water molecules
  - chemical cross-links like disulphide bonds ( $< 1nm$ ).
2. Figure 9 shows formation of a complex AB between molecule A and B. Explain why shapes of both molecules and chemical properties of both surfaces involved in the interactions are important. Explain, how nature is able to design matching molecular pairs, which bind very strongly to each other, but not to any other molecule inside a cell. Appendix B list chemical structure of amino acids involved in the interactions for those two proteins (marked on the Figure 9). (5p)  
 All interactions involved in protein-protein binding are short range. In addition they are specific in such way, that hydrophobic parts will only be attracted by other hydrophobic parts and not by charge or polar aa. To make two matching surfaces we need to have matching shapes - hand-glove type of fit and also matching chemical properties of both surfaces. In formed complex hydrophobic aa from both proteins are next to each other, those which form h-bonds must also be not more then a nm apart.



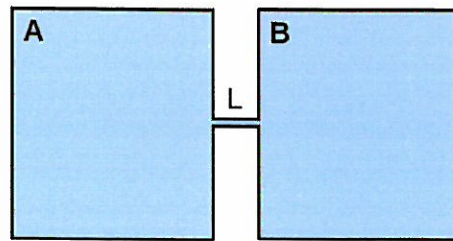


Figur 9: Binding between two protein molecules. Although protein-protein interactions occur over a large surface area, X-ray crystallography have shown that many protein-protein interfaces contain compact, centralized regions of residues - 'hot spots' - that are crucial for the interaction. The binding site is colored by atom type and the consensus binding site is outlined.

3. Denaturation is a process of "forced" unfolding of a protein molecule. Which of the following environmental changes is likely to enhance denaturation. Shortly explain why.
  - raising the temperature (2p)  
 this will increase strength of hydrophobic interactions and therefore promote folded state. Reducing the temperature might unfold the protein. Very large increase in temperature will also unfold proteins due to increased Brownian motion
  - replacing surrounding water with non-polar solvent (2p)  
 Polar solvent will destroy hydrophobic interactions and therefore denature the protein.
  - increasing amount of salt in solution (2p)  
weakens charge-charge interactions and therefore promotes denaturation
4. What is defined by **depletion force** and how this force is important for interaction between large protein molecules inside a cell. (4p)  
 depletion force in a attractive force between large objects (for example large globular proteins) in a presence of small molecules. Short range interaction. Entropic in origin. If two large molecules are separated, each of them is surrounded by a small depletion zone which is not accessible for small molecules. If two large molecules stick together, the total volume of that depletion zone is reduced and small molecules gain entropy. Inside the cell, depletion force will promote interactions between large protein molecules - helps large molecules to find each other.

### Question 3 Transport (20p)

1. Equation 13 (diffusion equation in 1D, Appendix A) describes how local concentration of dissolved molecules will change with time due to diffusion. Imagine two large containers connected through a narrow channel with a circular cross-section (radius: 100  $\mu\text{m}$ , length  $L = 1\text{ cm}$ ) as shown in Figure 10.  
 Container **A** contains 0.02M solution of Glucose and 0.01M solution of Ethanol in water.  
 Container **B** contains 0.02M solution of Ethanol in water.



Figur 10: Experimental setup

- What will be a **steady state** situation for the system shown above. Solve diffusion equation for a steady state situation, calculate and plot concentration profiles for Glucose and Ethanol inside the channel. (10p)

In the steady state situation the concentration profile inside the channel will not change with time. In this case the concentration inside the containers A and B will not change very much since there amount of glucose and ethanol inside the containers is much larger then what is moving through the channel. This will not be true over extensive time period. For steady state situation:

$$\begin{aligned}\frac{\partial c}{\partial t} &= D \frac{\partial^2 c}{\partial x^2} \\ 0 &= D \frac{\partial^2 c}{\partial x^2} \\ \frac{\partial c}{\partial x} &= C_1 \\ c(x) &= C_1 x + C_2\end{aligned}$$

If we define  $c_g^A$  as concentration of Glucose in A;  $c_g^B$  as concentration of Glucose in B;  $c_e^A$  as concentration of Ethanol in A;  $c_e^B$  as concentration of Ethanol in B; x-coordinate is zero for Then:

$$\begin{aligned}c_g(0) &= c_g^A \\ c_g(L) &= c_g^B \\ c_e(0) &= c_e^A \\ c_e(L) &= c_e^B\end{aligned}$$

Using those boundary conditions we get:

$$\begin{aligned}c_g(x) &= \frac{c_g^B - c_g^A}{L}x + c_g^A \\ c_e(x) &= \frac{c_e^B - c_e^A}{L}x + c_e^A\end{aligned}$$

- Will the concentration profile of Glucose inside the channel depend on the concentration of Ethanol inside the channel? (1p)  
NO
- Will the flux of Glucose molecules depend on the flux of Ethanol molecules. (1p)  
NO



- How will the concentration profiles and flux  $j$  through the channel depend on the channel width? (3p)  
 NO and NO: flux - net number of particles moving due to diffusion per unit area and unit time. So flux itself will not depend on the channel diameter, as long as it is small enough that steady state conditions apply. How much mass will be transported will depend on the channel cross-section.
- 2. What is defined by Reynolds number? What range of Reynolds number typically describe nano- and micro-fluidics devices. Calculate Reynolds number for a microfluidic device with a channel width of  $1 \times 10^{-6} \text{ m}$  and fluid velocity of  $1 \times 10^{-6} \text{ ms}^{-1}$ . What consequences do it have to the properties of water at those length scales. (5p)

$$\Re = \frac{vR\rho}{\eta} \quad (1)$$

Reynolds number is user to estimated ratio between viscous force and inertia for moving liquid. For  $\Re \ll 1$ , which is the case for micro and nanofluidic devices viscosity is dominating. This results in laminar flow, and mixing only due to diffusion. For given device

$$\Re = \frac{1 \times 10^{-6} \cdot 1 \times 10^{-6} \cdot 1 \times 10^3}{1 \times 10^{-3}} = 1 \times 10^{-6} \ll 1$$

#### Question 4 Entropic forces (10p)

At macro-scale, mechanical force is defined as a change in potential energy  $U$  with respect to some state variable  $x$ :

$$f = -\frac{dU}{dx}$$

- defined entropic force and list some examples; (4p)  
 defined similar to the mechanic force, but in this case we look at a change in free energy with respect to some state variable  $x$ . Force originate from the tendency of the system to increase its entropy, even at the cost of internal energy (still the free energy always goes down when system is doing work, e.g. a polymer chain contracts to equilibrium end to end distance, this includes increase in energy  $\Delta E$  and larger increase in term  $T\Delta S$ ). Examples include pressure in the ideal gas, osmotic pressure, hydrophobic interactions in water solution, depletion forces, electrostatic interactions in solution where both energy and entropy plays a role.
- which of those forces will be important for a living cell, explain how; (3p)
  - hydrophobic interactions - protein folding, formation of cell membranes, intermolecular interactions,
  - depletion forces - intermolecular interactions and molecular recognition
  - osmotic flow/pressure - cells need to maintain concentration gradients and work against osmotic pressure.
  - interaction between charged object inside the cell - short range of the interactions due to screening, attraction due to entropy gain of released counterions.
- What is a origin of repulsion force between two charged surfaces shown in Figure 11 when they are placed in water containing some dissolved NaCl. How would the situation be different in vacuum (no water and no salt). (3p)  
 Moving charged surfaces closer together will compere ion layers, reducing their entropy. System will try to oppose this with an entropic force which tries to push the plates

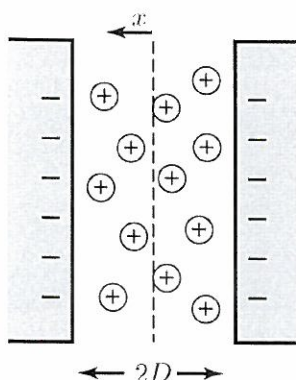


Figure 11: Repulsion between two charged surfaces

apart (in a similar way as gas under pressure tries to increase its volume). At larger separations this is not due to charge-charge interactions. At very small separation charge-charge interactions will also be important

### Question 5 Molecular Motors (10p)

Why is diffusion important in describing the behavior of molecular motors. Equation 64 (Appendix A) describes the velocity of idealized molecular motor based on S-ratchet concept (Fig 12).

Molecular motors move through diffusion (random walk) and use the supplied from the outside energy to control direction of that random motion.

1. Show that in a absence of external load, the motor speed will be:

$$v = \frac{2D}{L}$$

Hint: use  $e^{\bar{f}} = 1 + \bar{f} + \frac{1}{2}\bar{f}^2$ , with  $\bar{f} = \frac{fL}{k_B T}$  (3p)

$$\begin{aligned} v &= \left( \frac{fL}{k_B T} \right)^2 \frac{D}{L} \left( e^{fL/k_B T} - 1 - \frac{fL}{k_B T} \right)^{-1} \\ e^{fL/k_B T} &= 1 + \frac{fL}{k_B T} + \frac{1}{2} \left( \frac{fL}{k_B T} \right)^2 + \dots \\ v &= \left( \frac{fL}{k_B T} \right)^2 \frac{D}{L} \left( 1 + \frac{fL}{k_B T} + \frac{1}{2} \left( \frac{fL}{k_B T} \right)^2 + \dots - 1 - \frac{fL}{k_B T} \right)^{-1} \\ v &= \left( \frac{fL}{k_B T} \right)^2 \frac{D}{L} \left( \frac{1}{2} \left( \frac{fL}{k_B T} \right)^2 \right)^{-1} \\ v &= \frac{2D}{L} \end{aligned}$$

Motion from chemical energy is achieved by controlling direction of diffusion, so how fast things diffuse will limit the maximum speed of a molecular motor. It is diffusion of the moving parts in the motor which play a role, not the whole motor. If molecular motor is pulling, for example a vesicle, load comes from viscous friction. Therefore, in principle, motor is able to move very large cargo, but this will happen at low speed.

2. Calculate  $v$  for a motor making steps of 9nm. This motor is a protein molecule with a spherical shape and diameter of 20nm. (3p)

3. For a real molecular motor, what other factors will affect the speed at which it is moving. What is a typical source of energy for molecular motors found in cells and when they move a long the track pulling a load, what is this energy used for. (**4p**)

We first have to calculate  $D$  for this idealized motor:

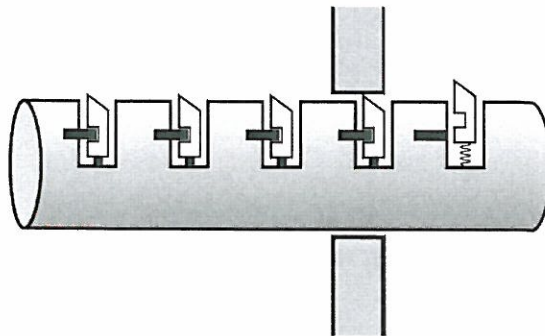
$$D\zeta = k_B T$$

$$D = \frac{k_B T}{6\pi\eta R} = \frac{4.1 \times 10^{-21}}{6\pi \times 10^{-3} \cdot 10 \times 10^{-9}} = 2 \times 10^{-11}$$

Then, maximum velocity of this motor will be:

$$v = \frac{4 \times 10^{-11}}{9 \times 10^{-9}} = 4 \times 10^{-3} \text{ ms}^{-1}$$

This speed will be slower for a real motor, slowed down for example by chemical reaction of getting the energy from ATP and by the presence of the load. The energy is used to combat viscous friction, and eventually the energy is converted into local increase in temperature (kinetic energy of surrounding water molecules). Not to increase potential or kinetic energy of moved cargo.



Figur 12: S-ratchet



## Appendix A: Equation Sheet

$$k_B = 1.38 \times 10^{-23} \text{J K}^{-1} \quad (2)$$

$$e = 1.6 \times 10^{-19} \text{Coul.} \quad (3)$$

$$\varepsilon_0 = 8.9 \times 10^{-12} \text{F m}^{-1} \quad (4)$$

$$v_{drift} = \frac{f}{\xi} \quad (5)$$

$$\xi = 6\pi\eta R \quad (6)$$

$$\xi D = k_B T \quad (7)$$

$$\lambda_X = \sqrt{2Dt} \quad (8)$$

$$\lambda_{3D} = \sqrt{6Dt} \quad (9)$$

$$\langle r^2 \rangle = NL_{seg}^2 \quad (10)$$

$$D = \frac{1}{\tau} \int_{-\infty}^{\infty} \frac{\Delta^2}{2} \rho(\Delta) d\Delta \quad (11)$$

$$2D\tau = \langle \Delta^2 \rangle \quad (12)$$

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} \quad (13)$$

$$j_s = -D \frac{\partial c}{\partial x} \quad (14)$$

$$\frac{\partial c}{\partial t} = -\frac{\partial j}{\partial x} \quad (15)$$

$$j_s = -P_s \Delta c \quad (16)$$

$$\frac{\partial c}{\partial t} = D \nabla^2 c \quad (17)$$

$$\vec{j} = -D \nabla c \quad (18)$$

$$c(\vec{r}, t) = \frac{N}{(4\pi Dt)^{3/2}} e^{-\frac{r^2}{4Dt}} \quad (19)$$

$$j = D \left( -\frac{dc}{dx} + \frac{q}{k_B T} \varepsilon c \right) \quad (20)$$

$$\Delta[\ln c] = -\frac{q}{k_B T} \Delta V \quad (21)$$

$$c(z) = C e^{\frac{-m_{eff} g z}{k_B T}} \quad (22)$$

$$j(r) = D \left( -\frac{dc}{dr} + \frac{r\omega^2 m_{eff}}{k_B T} c(r) \right) \quad (23)$$

$$c(r) = C e^{\frac{m_{eff} \omega^2 r^2}{2k_B T}} \quad (24)$$

$$v_{crit} = \frac{\eta}{\rho R} \quad (25)$$

$$f_{crit} = \frac{\eta^2}{\rho_m} \quad (26)$$

$$f_{fric} = \frac{\eta t^3 v}{R^2} \quad (27)$$

$$f_{inert} = \frac{\rho_m \ell^3 v^2}{R} \quad (28)$$

$$\Re = \frac{v R \rho}{\eta} \quad (29)$$

$$\frac{f}{A} = -G \frac{\Delta z}{d} \quad (30)$$

$$\frac{f}{A} = -\eta \frac{v}{d} \quad (31)$$

$$Q = \frac{\pi R^4 p}{8L\eta} \quad (32)$$

$$\frac{k_B T}{2} = \alpha \frac{\langle x^2 \rangle}{2} \quad (33)$$

$$S \equiv k_B \ln \Omega \quad (34)$$

$$T^{-1} = \left( \frac{dS}{dE} \right) \quad (35)$$

$$\Delta U = \Delta Q + \Delta W \quad (36)$$

$$\Delta S \geq \frac{\Delta Q}{T} \quad (37)$$

$$F_a \equiv E_a - TS_a \quad (38)$$

$$G_a \equiv E_a + pV_a - TS_a \quad (39)$$

$$\frac{P_1}{P_2} = e^{\frac{\Delta E}{k_B T}} \quad (40)$$

$$P_1 = \frac{1}{1 + e^{-\frac{\Delta E}{k_B T}}} \quad (41)$$

$$P_2 = \frac{1}{1 + e^{\frac{\Delta E}{k_B T}}} \quad (42)$$

$$\tau^{-1} = C e^{\frac{-\Delta E_1}{k_B T}} \left( 1 + e^{\frac{-\Delta E}{k_B T}} \right) \quad (43)$$

$$\Delta F = \Delta F_0 - f \Delta z \quad (44)$$

$$Z = \sum_j e^{-E_j/k_B T} \quad (45)$$

$$p_{equil} = c_{osm} k_B T \quad (46)$$

$$c_{osm} = \varphi M c \quad (47)$$

$$\Sigma = \frac{Rp}{2} \quad (48)$$

$$\ell_B \equiv \frac{e^2}{4\pi\varepsilon k_B T} \quad (49)$$

$$\bar{V}(x) = \frac{cV(x)}{k_B T} \quad (50)$$

$$c_+(x) = \frac{2\pi\ell_B \left( \frac{\sigma_q}{\epsilon} \right)^2}{\left( 1 + 2\pi\ell_B \frac{\sigma_q}{\epsilon} x \right)^2} \quad (51)$$

$$x_0 = \left( \frac{c}{2\pi\ell_B \sigma_q} \right) \quad (52)$$

$$\frac{d^2 \bar{V}}{dx^2} = -4\pi\ell_B c_0 e^{-\bar{V}} \quad (53)$$

$$\lambda_D = (8\pi\ell_B c_\infty)^{-\frac{1}{2}} \quad (54)$$

$$V(x) = -\frac{\sigma_q \lambda_D}{\varepsilon} e^{-\frac{x}{\lambda_D}} \quad (55)$$

$$f = 2k_B T b^2 r \quad (56)$$

$$b^2 \propto \frac{1}{nl^2} \quad (57)$$

$$\langle z/L_{tot} \rangle = \tanh \left( f L_{seg}^{(1d)} / k_B T \right) \quad (58)$$

$$\langle z/L_{tot} \rangle = \coth(f L_{seg}/k_B T) - (f L_{seg}/k_B T)^{-1} \quad (59)$$

$$\langle z/L_{tot} \rangle = \frac{\sinh \alpha}{\sqrt{\sinh^2 \alpha + e^{-4\gamma}}} \quad (60)$$

$$\alpha \equiv \frac{f\ell}{k_B T} \quad (61)$$

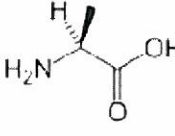
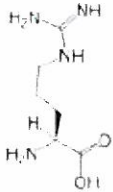
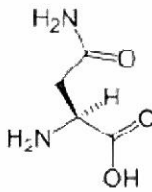
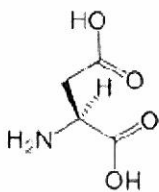
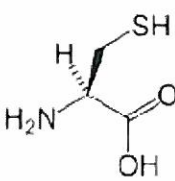
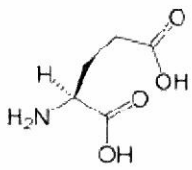
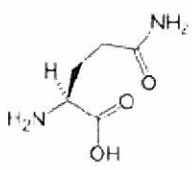
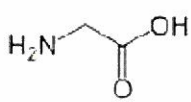
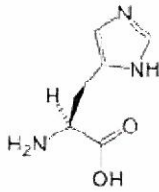
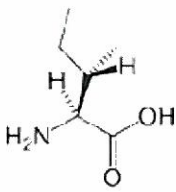
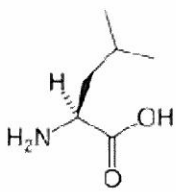
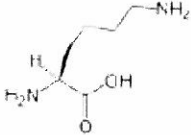
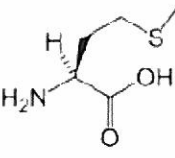
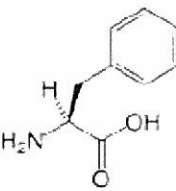
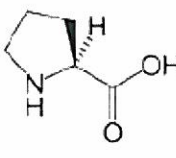
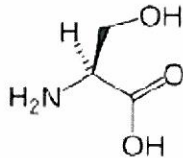
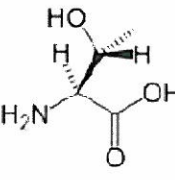
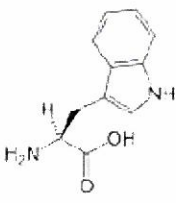
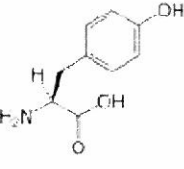
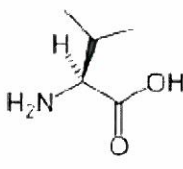
$$j(x) = c v_{drift} - D \frac{dc}{dx} \quad (62)$$

$$j^{(1D)} = -MD \left( \frac{dP}{dx} + \frac{1}{k_B T} P \frac{dU_{tot}}{dx} \right) \quad (63)$$

$$c = \left( \frac{fL}{k_B T} \right)^2 \frac{D}{L} \left( c^{fL/k_B T} - 1 - \frac{fL}{k_B T} \right)^{-1} \quad (64)$$



## Appendix B: Chemical Structures of Amino Acids

			
L-Alanine (Ala / A)	L-Arginine (Arg / R)	L-Asparagine (Asn / N)	L-Aspartic acid (Asp / D)
			
L-Cysteine (Cys / C)	L-Glutamic acid (Glu / E)	L-Glutamine (Gln / Q)	Glycine (Gly / G)
			
L-Histidine (His / H)	L-Isoleucine (Ile / I)	L-Leucine (Leu / L)	L-Lysine (Lys / K)
			
L-Methionine (Met / M)	L-Phenylalanine (Phe / F)	L-Proline (Pro / P)	L-Serine (Ser / S)
			
L-Threonine (Thr / T)	L-Tryptophan (Trp / W)	L-Tyrosine (Tyr / Y)	L-Valine (Val / V)