Homework No. 1

Fundamentals of AFM: Part I

Lectures: P1_Wk1_L1 - P1_Wk1_L6

Problem 1: Ion-ion Interactions

Two Na ions are dissolved in ethanol which has a dielectric constant of 24.

Q1.1. What is the separation between these two ions when they realize a force of 1 nN (1nN=1x10^{-9} N)?

$a)$ 0.48 nm $c)$ 98 pm
$b)$ 1.0 nm $d)$ 256 pm

Correct answer is c).

Solution:

$$F = \frac{1}{4\pi\varepsilon_o}\frac{1}{\kappa}\frac{q_1 q_2}{r^2} = \frac{1}{4\pi \cdot 8.85\times 10^{-12}\, C^2/Nm^2}\frac{1}{24}\frac{\left(1.602\times 10^{-19}C\right)^2}{r^2} = 1\times 10^{-9}\,N$$

$$1\times 10^{-9} = 3.746\times 10^{8}\cdot\frac{\left(1.602\times 10^{-19}\right)^2}{r^2} = \frac{9.60\times 10^{-30}}{r^2}$$

$$r = 9.8\times 10^{-11}m = 98\,pm$$

Q1.2. How much energy is stored in the system when the two ions are brought to this separation?

$$a) \quad -2.4\times10^{-18}\,J \qquad c) \quad 6.3\times10^{-20}\,J$$
$$b) \quad 9.8\times10^{-20}\,J \qquad d) \quad 1.6\times10^{-19}\,J$$

Correct answer is b).

Solution:

$$U_{electr} = \frac{1}{4\pi\varepsilon_o}\frac{1}{\kappa}\frac{q_1q_2}{r} = \frac{1}{4\pi\cdot 8.85\times10^{-12}\,C^2/Nm^2}\cdot\frac{1}{24}\cdot\frac{\left(1.602\times10^{-19}C\right)^2}{98\times10^{-12}m}$$
$$= 3.746\times10^8\cdot\frac{\left(2.566\times10^{-38}\right)}{98\times10^{-12}}N\cdot m = +9.81\times10^{-20}\,J$$

Q1.3. If the ions are in ethanol held at 300 K, is it likely they will ever feel a repulsive force of 1 nN?

a) Yes, thermal energies are more than sufficient to overcome the electrostatic energy required for the specified configuration
b) Possibly, since thermal energies are comparable to the electrostatic energy required for the specified configuration
c) No, thermal energies are too small to overcome the electrostatic energy required for the specified configuration

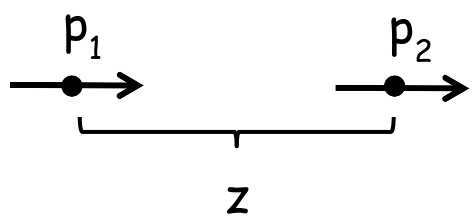
Solution:

$$\text{Thermal energy available} \approx k_BT = \left(1.38\times10^{-23}\,J/K\right)\cdot\left(300K\right) = 4.14\times10^{-21}\,J$$
$$\frac{U_{electr}}{k_BT} = \frac{9.8\times10^{-20}\,J}{4.14\times10^{-21}\,J} \simeq 24$$

The correct answer is c) since the electrostatic energy required to assemble the two ions is ~24 times greater than the typical thermal energies available.

Problem 2: Dipole-dipole Interactions

What is the energy of interaction of two permanent dipoles of strength 1D if they are separated by 0.5 nm in vacuum? Assume the dipoles are aligned as shown below.



a) 2.4×10^{-18} J; repulsive

b) 9.8×10^{-20} J; attractive

c) 6.3×10^{-20} J; repulsive

d) 1.6×10^{-21} J; attractive

Correct answer is d).

Solution:

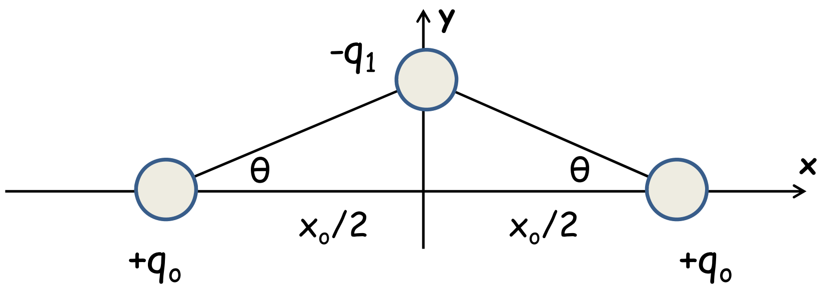
$$U(z) = -\frac{p_1 p_2 \left[2\cos(\theta_1)\cos(\theta_2) - \sin(\theta_1)\sin(\theta_2)\cos(\phi)\right]}{4\pi\kappa\varepsilon_0 z^3}$$

$$\theta_1 = 0; \quad \theta_2 = 0; \quad \phi = 0; \quad p_1 = p_2 = 1D = 3.33 \times 10^{-30}\, Cm; \; \kappa = 1$$

$$U(z) = -\frac{p_1 p_2 [2]}{4\pi\varepsilon_0} \frac{1}{z^3} = -9 \times 10^9\, Nm^2/C^2 \cdot \frac{2\left(3.33 \times 10^{-30} Cm\right)^2}{(0.5 \times 10^{-9})^3} = -1.6 \times 10^{-21} J$$

Problem 3. Simple model for chemical bond

A very simple electrostatic model for a chemical bond that forms between two atoms is given below.



The two charges $+q_o$ are fixed at a distance x_o apart. These two charges might represent the positive charge on the nucleus of each atom. The negative charge q_1 might represent electrons that (in this simple model) are constrained to move along the perpendicular bisector (y-axis) as shown in the diagram. The angle θ is constrained such that $-\pi/2<\theta<\pi/2$. In what follows, assume that all charges are stuck down as shown above.

Q3.1 By inspection, what is the interaction potential energy for the charge configuration drawn above?

$$a)\ U = \frac{1}{4\pi\varepsilon_o}\left(\frac{q_o^2}{x_o} - \frac{2q_1q_o}{\sqrt{\left(x_o^2/4 + y^2 \right)}} \right)$$

$$c)\ U = \frac{1}{4\pi\varepsilon_o}\left(-\frac{q_o^2}{x_o} + \frac{2q_1q_o}{\sqrt{\left(x_o^2/4 + y^2 \right)}} \right)$$

$$b)\ U = \frac{1}{4\pi\varepsilon_o}\left(\frac{q_o^2}{x_o} + \frac{2q_1q_o}{\sqrt{\left(x_o^2/4 + y^2 \right)}} \right)$$

$$d)\ U = \frac{1}{4\pi\varepsilon_o}\left(\frac{q_o^2}{x_o^2} - \frac{2q_1q_o}{\left(x_o^2/4 + y^2 \right)} \right)$$

Correct answer is a).

Q3.2 Rewrite the answer to Q3.1 above in terms of θ?

$$a)\ \frac{1}{4\pi\varepsilon_o}\frac{q_o^2}{x_o^2}\left(1+\frac{4q_1}{q_o}\cos\theta\right)$$

$$b)\ \frac{1}{4\pi\varepsilon_o}\frac{q_o^2}{x_o^2}\left(1-\frac{4q_1}{q_o}\cos\theta\right)$$

$$c)\ \frac{1}{4\pi\varepsilon_o}\frac{q_o^2}{x_o}\left(1+\frac{4q_1}{q_o}\cos\theta\right)$$

$$d)\ \frac{1}{4\pi\varepsilon_o}\frac{q_o^2}{x_o}\left(1-\frac{4q_1}{q_o}\cos\theta\right)$$

Correct answer is d).

Solution:

$$U=\frac{1}{4\pi\varepsilon_o}\left(\frac{q_o^2}{x_o}-\frac{2q_1q_o}{\sqrt{\left(x_o^2/4+y^2\right)}}\right)=\frac{1}{4\pi\varepsilon_o}\left(\frac{q_o^2}{x_o}-\frac{2q_1q_o}{x_o}\cdot\frac{x_o}{\sqrt{\left(x_o^2/4+y^2\right)}}\right)$$

$$\sin\theta=\frac{y}{\sqrt{\left(x_o^2/4+y^2\right)}}\qquad\cos\theta=\frac{x_o/2}{\sqrt{\left(x_o^2/4+y^2\right)}}$$

$$=\frac{1}{4\pi\varepsilon_o}\left(\frac{q_o^2}{x_o}-\frac{4q_1q_o\cos\theta}{x_o}\right)=\frac{1}{4\pi\varepsilon_o}\frac{q_o^2}{x_o}\left(1-\frac{4q_1}{q_o}\cos\theta\right)$$

Q3.3 In this simple model, the range of values for the ratio of q_1/q_o has not been specified. What restriction must be placed on q_1/q_o for U to have a negative value?

a) $\frac{q_1}{q_o} < \frac{1}{2}$

b) $q_1 = q_o$

c) $\frac{q_1}{q_o} > \frac{1}{2}$

d) $\frac{q_1}{q_o} > \frac{1}{4\cos\theta}$

Correct answer is d).

Solution:

$$U = \frac{1}{4\pi\varepsilon_o}\frac{q_o^2}{x_o}\left(1 - \frac{4q_1}{q_o}\cos\theta\right)$$

$$for\, U < 0, \quad \left(1 - \frac{4q_1}{q_o}\cos\theta\right) < 0 \Rightarrow \frac{4q_1}{q_o}\cos\theta > 1$$

$$\frac{q_1}{q_o} > \frac{1}{4\cos\theta}$$

The ratio of q_1/q_o to make U negative depends on θ.

Q3.4 For a given q_o, what is the value of θ for the system to have U<0 with the minimum value for q_1?

a) Θ=0°
b) Θ=30°
c) Θ=45°
d) Θ=60°
e) Θ=90°

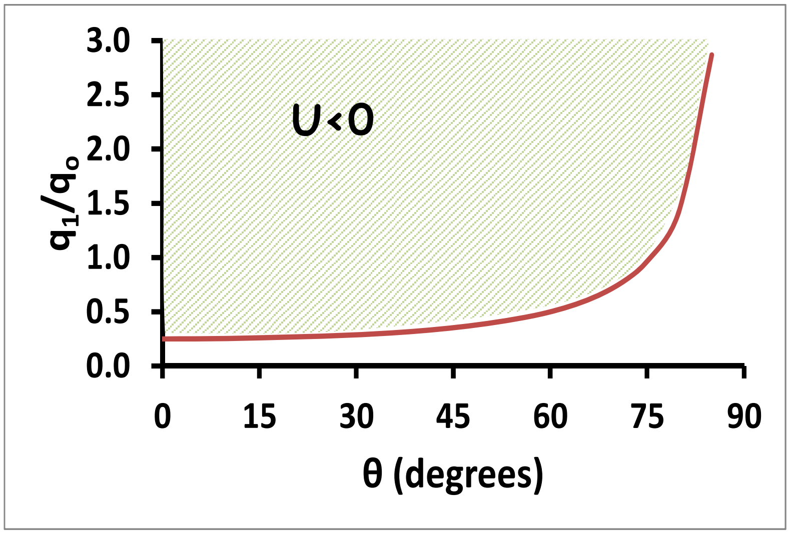
Correct answer is a).

Solution:

There are many ways to arrive at this answer. We showed above that the condition

$$\frac{q_1}{q_o} > \frac{1}{4\cos\theta}$$

is required to make U negative. Perhaps a simple sketch of q_1/q_o vs θ is the best way to "see" that θ =0 minimizes the value of q_1 for a given q_o. The required plot is shown below.



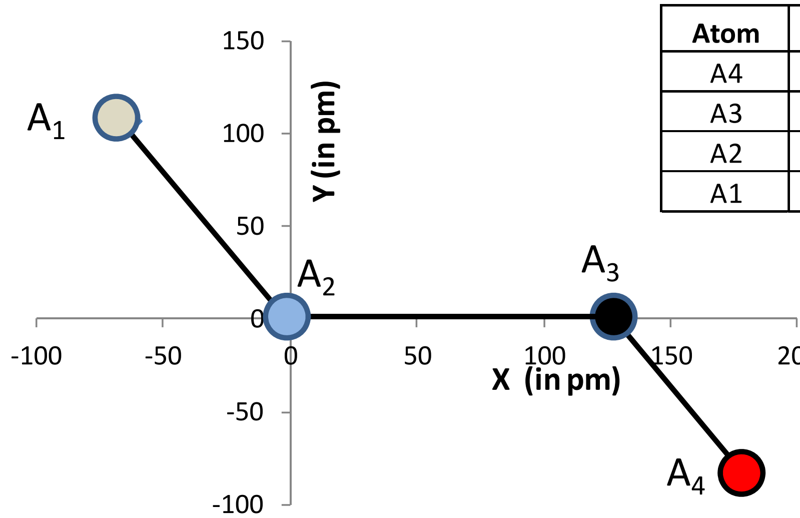
Alternatively, what value of θ maximizes the denominator in the above equation? This angle will then give the minimum value for q_1/q_o while maintaining the condition U<0. The answer is θ=0; cos θ=1 giving

$$q_1 > \frac{1}{4} q_o \,.$$

From this discussion we might conclude that if we confine a negative charge along a line "between" two positive charges, the electrostatic potential energy of the system can be made less than zero. This does not say anything about whether the system is in stable equilibrium, it just says that the potential energy stored in the system of charges is less than when the charges were infinitely far apart.

Problem 4. Dipole moment of molecule

Four atoms are arranged in a hypothetical planar molecule as shown in the Figure below. The partial electronic charge on each atom can be computed from a quantum chemistry calculation and these partial charges, as well as the atom co-ordinates, are given in the table. (1 pm = 1 x10^{-12} m).



Atom	x (pm)	y (pm)	δq (e^-)
A4	190	-90	0.20
A3	125	0	-0.33
A2	0	0	0.48
A1	-65	115	-0.35

Q4.1. What is the component of the dipole moment (in Debye) of this molecule in the x-direction?

a) 0.53 D
b) -0.67 D
c) 0.94 D
d) 1.58 D

Correct answer is c).

Solution:

$$p_x = \sum_{i=1}^{4} x_i \delta q_i = 19.5\, pm \cdot e^- \times \frac{1\times10^{-12}\, m}{pm} \times \frac{1.6\times10^{-19}\, C}{e^-}$$

$$= 3.12\times10^{-30}\, Cm \times \frac{1D}{3.335\times10^{-30}\, Cm} = 0.94\ D$$

Q4.2. What is the component of the dipole moment (in Debye) of the molecule in the y-direction?

a) -1.37 D
b) 3.68 D
c) 0.44 D
d) -2.80 D

Correct answer is d).

Solution:

$$p_y = \sum_{i=1}^{4} y_i \delta q_i = -58.3\, pm \cdot e^- \times \frac{1\times10^{-12}\, m}{pm} \times \frac{1.6\times10^{-19}\, C}{e^-}$$

$$= -9.33\times10^{-30}\, Cm \times \frac{1D}{3.335\times10^{-30}\, Cm} = -2.80\ D$$

Q4.3. What is the magnitude of the dipole moment (in Debye) for this molecule?

a) 4.79 D
b) 1.80 D
c) 2.95 D
d) 3.68 D

Correct answer is c).

Solution:

$$\left|\vec{p}\right| = \sqrt{p_x^2 + p_y^2} = \sqrt{(0.94)^2 + (-2.80)^2} = \sqrt{8.72}\ D = 2.95\ D$$