Homework No. 1

Fundamentals of AFM: Part I

Lectures: P1_Wk1_L1 - P1_Wk1_L6

Problem 1:

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*

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

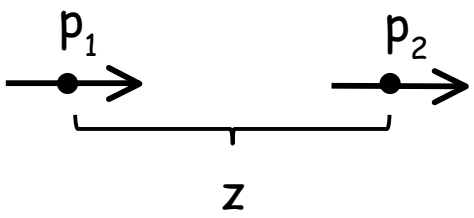
a) $-2.4\times10^{-18}J$ *c*) $6.3\times10^{-20}J$
b) $9.8\times10^{-20}J$ *d*) $1.6\times10^{-19}J$

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

Problem 2:

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

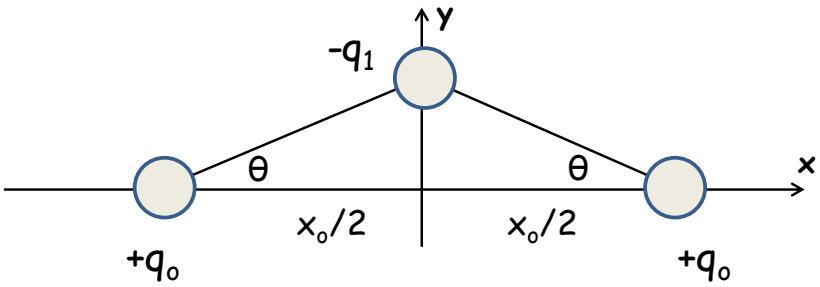
b) 9.8×10^{-20} J; attractive

c) 6.3×10^{-20} J; repulsive

d) 1.6×10^{-21} J; attractive

Problem 3.

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?

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

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

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

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

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

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

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

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

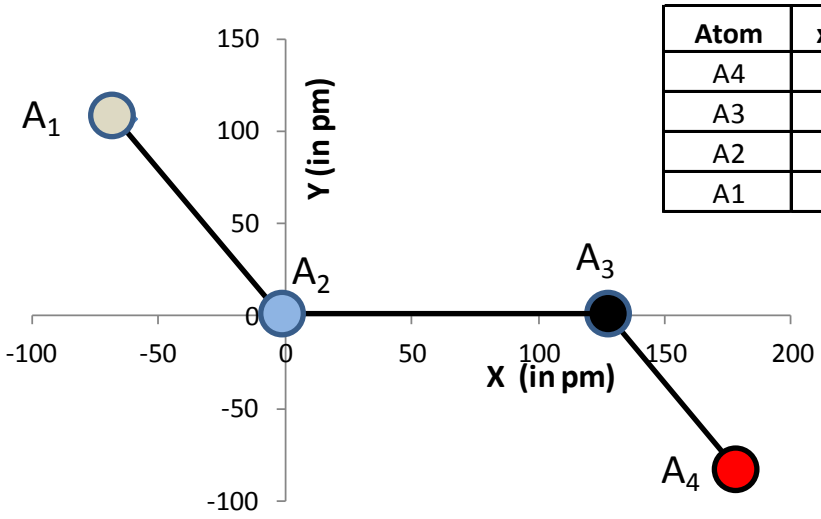
d) $\frac{q_1}{q_o} > \frac{1}{4\cos\theta}$

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

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

Problem 4.

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

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

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