Solution to FMS Homework 5, SS 2017

1. **(a)** Using the ionic radii data in your textbook, calculate the coulombic force of attraction between Na^+ and Cl^- in NaCl. You may want to check the structure of NaCl to figure out the separation distance between the ions.
   (b) What is the repulsive force in this case?

SOLUTION:

Coulombic force of attraction between two ions:

$$F_c = \frac{-K}{a^2}$$

$$K = K_0 (Z_1 q)(Z_2 q)$$

q: charge of single e, 1.6×10^{-19} C

K_0: proportionality constant 9×10^9 V·m/C

Z_1, Z_2 : Valence

(a) For NaCl: $r_{Na^+} = 0.098$ nm

$r_{Cl^-} = 0.181$ nm

$$a = r_{Na^+} + r_{Cl^-} = 0.098 + 0.181 = 0.278 \text{ nm}$$

$$F_c = -\frac{K_0 (Z_1 q)(Z_2 q)}{a^2}$$

$$= -\frac{9\times10^9 \text{ V·m/C } (+1)(1.6\times10^{-19} C)(-1)(1.6\times10^{-19} C)}{(0.0278\times10^{-9} m)^2}$$

$$= \underline{2.98\times10^{-9} N}$$

(b) $F_c + F_R = 0 \Rightarrow F_R = \underline{-2.98\times10^{-9} N}$

2. **(a)** A common way to describe the bonding energy curve for secondary bonding is the "6–12" potential, which states that

$$E = -\frac{K_A}{a^6} + \frac{K_R}{a^{12}},$$

where K_A and K_R are constants for attraction and repulsion, respectively. This relatively simple form is a quantum mechanical result for this relatively simple bond type. Given $K_A = 10.37 \times 10^{-78} J \cdot m^6$ and $K_R = 16.16 \times 10^{-135} J \cdot m^{12}$, calculate the bond energy and bond length for argon.

(b) Plot E as a function of a over the range 0.33 to 0.80 nm.

Solution:

(a) At equilibrium: $\frac{dE}{da} = 0$, $\left(\frac{dE}{dr} = 0\right)$

$$\left(\frac{dE}{da}\right)_{a=a_0} = 0 = \frac{6K_A}{a_0^7} - \frac{12K_B}{a_0^{13}}$$

$$\Rightarrow a_0 = \left(2\frac{K_B}{K_A}\right)^{1/6}$$

$$= \left(2 \times \frac{16.16\times10^{-135}}{10.37\times10^{-78}}\right)^{1/6} m$$

$$= 0.382 \times 10^{-9} m = 0.382 \text{ nm}$$

$$\Rightarrow E_{a=a_0} = -\frac{K_A}{(0.382 \text{ nm})^6} + \frac{K_B}{(0.382 \text{ nm})^{12}}$$

$$= -\frac{10.37\times10^{-78} J\cdot m^6}{(0.382\times10^{-9} m)^6} + \frac{16.16\times10^{-135} J\cdot m^{12}}{(0.382\times10^{-9} m)^6}$$

$$= -1.66 \times 10^{-21} J$$

For 1 mole of Ar,

$$E = -1.66 \times 10^{-21} J/\text{bond} \times 6.02 \times 10^{23} \frac{\text{bonds}}{\text{mole}}$$

$$= -0.999 \times 10^3 J/\text{mol}$$

$$= -0.999 \text{ kJ/mol}$$

(b) Based on the equation in (a)

$$E = \left[-\frac{(10.37\times10^{-78} J\cdot m^6)}{a^6} + \frac{(16.16\times10^{-135} J\cdot m^{12})}{a^{12}} \right]$$

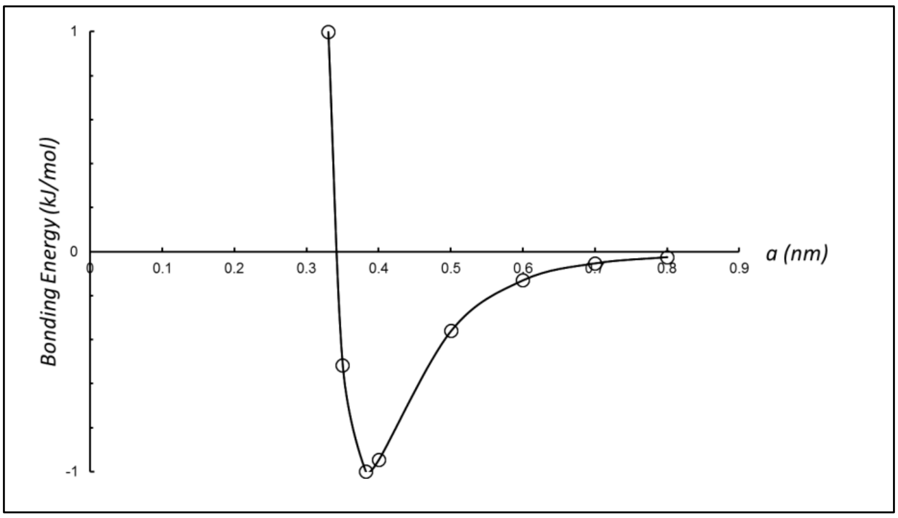
$$\times 6.023\times10^{23}\ mol^{-1}$$

So, we design a series of data in the given range between 0.33 and 0.80 of a:

You can tabulate the data in Excel:

a	E bonding
0.33×10^{-9} m	+0.999 kJ/mol
0.35 × "	−0.517 "
0.382 × "	−0.999 "
0.4 × "	−0.945 "
0.5 × "	−0.360 "
0.6 × "	−0.129 "
0.7 × "	−0.052 "
0.8 × "	−0.024 "

Use Excel or Origin to generate a professional plot, like what I did below.



3. The net potential energy between two adjacent ions, E_N, may be represent by the sum of Equations 2.9 and 2.11, that is,

$$E_n = -\frac{A}{r} + \frac{B}{r^n}$$

Calculate the bonding energy E_0 in terms of the parameters A, B, and n using the following procedure:

1) Different E_N with respect to r, and then set the resulting expression equal to zero, since the curve of E_N versus r is a minimum at E_0.
2) Solve for r in terms A, B, and n, which yields r_0, the equilibrium interionic spacing.
3) Determine the expression for E_0 by substitution of r_0 into Equation 2.17

Solution

1) 用E_N对r微分并使其表达式为0。

就可以了。挺简单的问题呀..

$$0 = \frac{dE_N}{dr} = \frac{d(-\frac{A}{r})}{dr} + \frac{d(\frac{B}{r^n})}{dr}$$

这样会有以A,B,n表示的r为变量的方程！

2) 求出r_0，把$r = r_0$带入

这样，r_0就可以用A,B,n表示

3) $E_N = -\frac{A}{r} + \frac{B}{r^n}$

r_0 r_0

就OK了！

带入r_0，$E_N = E_0$

4. For the Na^+-Cl^- ion pair, attractive and repulsive energies E_A and E_R, respectively, depend on the distance between the ions r, according to

$$E_A = -\frac{1.436}{r}$$

$$E_R = \frac{7.32 \times 10^{-6}}{r^8}$$

For these expressions, energies are expressed in electron volts per Na^+-Cl^- pair, and r is the distance in nanometers. The net energy E_N is just the sum of the two expressions above.

(a) Superimpose on a single plot E_N, E_R, and E_A versus r up to 1.0 nm.
(b) On the basis of this plot, determine (i) the equilibrium spacing r_0 between the Na^+ and Cl^- ions, and (ii) the magnitude of the bonding energy E_0 between the two ions.
(c) Mathematically determine the r_0 and E_0 values using the solutions to Problem 2.14 and compare these with the graphical results from part (b).

(a) Superimpose 指的是叠加，
这个题目是让你在一张图上画出
EN, ER, 和 EA，横坐标为离子
间距，最大值为 1.0 nm.
这个题目是个很好的锻炼！！！
有了函数 y=f(x)，你会不会
用电脑绘制出函数图形来呢？
而且需要把3个函数放在一张图
里面。有很多不错的软件可以完成这个

2维，而且能够非常professional地进行标注。最常用，最简单的软件就是Microsoft Excel，但它作出的图一般不是最漂亮。推荐用Origin这个软件，比较professional。

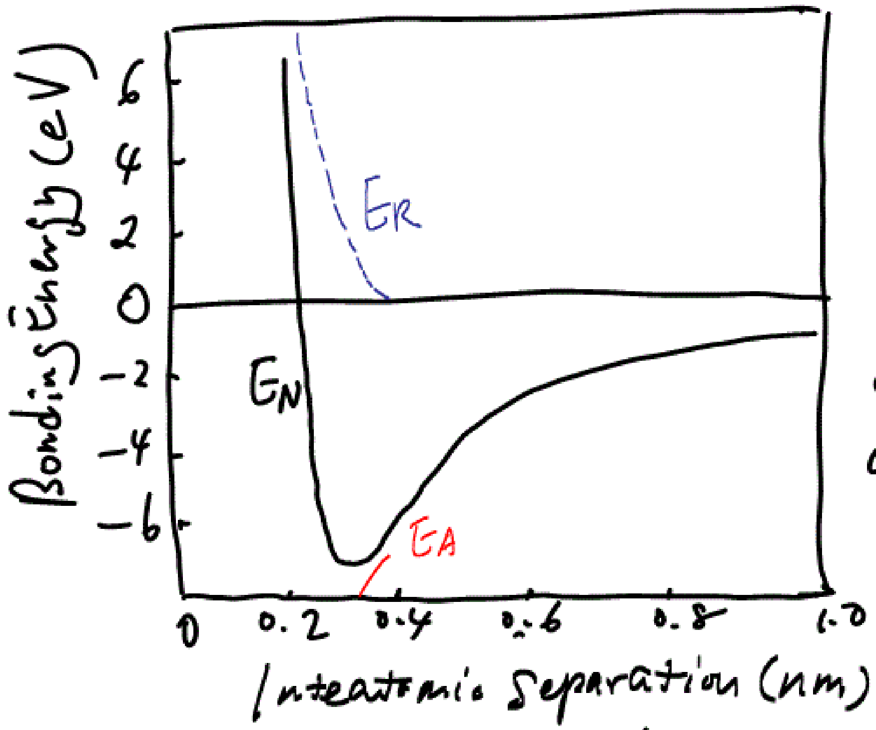
作图的时候你首先得找准数据。

例如：

数据的越密，你的曲线越平滑

r	E_A	E_R	E_N
0 0.1 0.2 ⋮ 1.0	$-\frac{A}{r}$ 有公式	$\frac{B}{r^n}$ 有公式	E_A+E_R 这个是由前面的数据用电脑自动算出来

然后你就可以用电脑画出这些函数了。用散点，然后拟合，或者用曲线均可。记住，不同的函数E_A，E_R，E_N要用不同的颜色。坐标轴要标注，要有图例。我给你们用手画个例子啊，你们用电脑应该比这漂亮。



类似这样的图。我画的不好，给你们做个参考。

(b) 从图中尽可能读出 $r_0 = \ldots$ nm

$E_0 = \ldots$ eV

(c) 2.14 最后一问不是求出 E_0 怎么用 A、B、n 表示了么。
现在 A、B、n 都已知，带进去，
算出 r_0 和 E_0，并与 (b) 从图中
读出的数据比较。

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于二教205办公室