T-L 9-41 (Sodium Chloride)

a) Electrostatic potential energy of Na^+ & Cl^- at their equilibrium separation $R_0 = 0.24nm$ (assuming point charges

$$U_{ele} = \frac{-1}{4\pi\epsilon_0}\frac{q_1 q_2}{r} = -9.61\times10^{-19}\text{ Joules} = \boxed{-6eV}$$

where I've assumed each ion has a single charge (singly ionized).

b) What is the energy of repulsion at this separation?

- Let me first write down some numbers for NaCl.
- Dissociation energy: $E_D =$ ~~4.6~~ $4.26eV$
- Net ionization energy: $E_{ion} = 1.53eV$
- Coulomb potential at 0.24nm: $U_{ele} = -6eV$
- Exclusion energy due to Pauli principle: $E_{ex} = \frac{A}{r^n}$, $A=?$, $n=?$
- Now, I'll follow example 9-1 in the book. The total potential energy at infinite distance apart is the net ionization energy needed to form Na^+ & Cl^-, which is 1.53eV.
- So the net Coulomb potential energy is

$$U_c = \frac{-kq^2}{r} + 1.53eV = -6eV + 1.53eV$$

$$U_c = -4.47eV$$

- Since the measured dissociation energy is 4.26eV, the potential energy due to the exclusion principle must be

$$E_{ex} = 4.47eV - \text{~~4.26~~ } 4.26eV =$$

$$\boxed{E_x = 0.21eV}$$

→

c) Now, how do I determine the parameters "n" and "A" in the formula $E_{ex} = \frac{A}{r^n}$?

- From the graph in Fig 9-2b, the coulomb attraction ~~repulsion~~ energy equals the exclusion principle repulsion energy when $r = r_1 = 0.14\text{nm}$. That is

$$\frac{A}{r_1^n} = \frac{ke^2}{r_1}$$

plugging in $r_1 = 0.14\text{nm}$

☺ $$\frac{A}{r_1^n} = 10.3\text{eV}$$

- We also know that the exclusion repulsion energy must be 0.21 eV at the equilibrium separation, from parts (a) & (b) of this problem. That is:

☹ $$\frac{A}{r_0^n} = 0.21\text{eV}$$

, where $r_0 = 0.24\text{nm}$

- Now combining ☺ & ☹ gives

$$\frac{\frac{A}{r_0^n}}{\frac{A}{r_1^n}} = \frac{0.21\text{eV}}{10.3\text{eV}}$$

$$\log\left[\left(\frac{r_1}{r_0}\right)^n = \frac{0.21}{10.3}\right]$$

$$n = \log\left[\frac{0.21}{10.3}\right] / \log\left[\frac{r_1}{r_0}\right] = 7.22$$

→

- If $n = 7.22$, then we can find A using either  or 

$$A = (0.21\,\text{eV})(0.24\,\text{nm})^{7.22}$$

- This has bizarre units. I'll round to $n = 7$.

$$A = (0.21\,\text{eV})(0.24\,\text{nm})^{7}$$

$$A = 1.5 \times 10^{-87}\ \text{kg}\,\text{m}^{9}/\text{s}^{2}$$

- The units are strange, but this is an approx. formula.