Problem 1

Calculate the lattice constant and binding energy of NaCl ions if the ions are doubly ionized (q=2 instead of 1).

Solution

We know from Charles Kitell's Introduction to Solid State physics equation 3.18 that:

$$U_{tot} = N(z\lambda e^{-\frac{R}{\rho}} - \frac{\alpha q^2}{R})$$

Now to solve for the equilibrium position R_o, we find the minimum of the energy with respect to R, $\frac{dU}{dR} = 0$:

$$R_o^2 e^{-\frac{R_o}{\rho}} = \frac{\rho \alpha q^2}{z\lambda}$$

Using the values $z\lambda = 1.05 \times 10^{-8} ergs = 1.05 \times 10^{-15}$ J Å and $\rho = 0.321$Å and $\alpha = 1.747565$, and substituting q^2 for $\frac{q^2}{4\pi\epsilon_o}$ we find that:

$$\frac{q^2}{4\pi\epsilon_o}\Big|_{q=1} = 2.307077 \times 10^{-18} J\AA$$
$$\frac{q^2}{4\pi\epsilon_o}\Big|_{q=2} = 9.228309 \times 10^{-18} J\AA$$

Therefore we obtain:

$$R_o^2 e^{-\frac{R_o}{0.321\AA}}\Big|_{q=1} = \frac{0.321\AA(1.747565)(2.307077 \times 10^{-18} J\AA)}{1.05 \times 10^{-15} J\AA} = 0.00123256\AA^2$$

$$R_o^2 e^{-\frac{R_o}{0.321\AA}}\Big|_{q=2} = \frac{0.321\AA(1.747565)(9.228309 \times 10^{-18} J\AA)}{1.05 \times 10^{-15} J\AA} = 0.00493026\AA^2$$

Solving for R_o yeilds:

$$\boxed{R_o\Big|_{q=1} = 2.81463\AA}$$

$$\boxed{R_o\Big|_{q=2} = 2.21616\AA}$$

The binding energy per atom is given by:

$$\frac{U_{tot}}{N} = -\frac{\alpha q^2}{R_o}(1 - \frac{\rho}{R_o})$$

Therefore we find:

$$\frac{U_{tot}}{N}\Big|_{q=1} = -\frac{1.747565(2.307077 \times 10^{-18} J\AA)}{2.81463\AA}(1 - \frac{0.321\AA}{2.81463\AA})$$
$$\frac{U_{tot}}{N}\Big|_{q=2} = -\frac{1.747565(9.228309 \times 10^{-18} J\AA)}{2.21616\AA}(1 - \frac{0.321\AA}{2.21616\AA})$$

$$\boxed{\frac{U_{tot}}{N}\Big|_{q=1} = -7.92eV}$$

$$\boxed{\frac{U_{tot}}{N}\Big|_{q=2} = -38.8eV}$$

Problem 2

Suppose you were abe to permeate space between ions in an ionic crystal with a dielectric ($\epsilon = 81$ like in water). This reduces the Coulomb interaction by $\frac{1}{\epsilon}$. Calculate the lattice constant and binding energy of NaCl in ths situation. Compare the binding energy per atom with the approximate thermal energy (kT) at room temperature.

Solution

Similar to before, we have the values $z\lambda = 1.05 \times 10^{-8} ergs = 1.05 \times 10^{-15}$ J Å and $\rho = 0.321$Å and $\alpha = 1.747565$, and substituting q^2 for $\frac{q^2}{4\pi\epsilon_o}$ we find that:

$$\frac{q^2}{4\pi\epsilon_o\epsilon}\Big|_{q=1} = 2.848244 \times 10^{-20} J\mathring{A}$$

Therefore we obtain:

$$R_o^2 e^{-\frac{R_o}{0.321\mathring{A}}}\Big|_{q=1} = \frac{0.321\mathring{A}(1.747565)(2.848244 \times 10^{-20} J\mathring{A})}{1.05 \times 10^{-15} J\mathring{A}} = 0.000015216\mathring{A}^2$$

Solving for R_o yeilds:

$$\boxed{R_o\Big|_{q=1} = 4.5309\mathring{A}}$$

The binding energy per atom is given by:

$$\frac{U_{tot}}{N} = -\frac{\alpha q^2}{R_o}(1 - \frac{\rho}{R_o})$$

Therefore we find:

$$\frac{U_{tot}}{N}\Big|_{q=1} = -\frac{1.747565(2.307077 \times 10^{-18} J\mathring{A})}{2.81463\mathring{A}}(1 - \frac{0.321\mathring{A}}{2.81463\mathring{A}})$$

$$\frac{U_{tot}}{N}\Big|_{q=2} = -\frac{1.747565(9.228309 \times 10^{-18} J\mathring{A})}{2.21616\mathring{A}}(1 - \frac{0.321\mathring{A}}{2.21616\mathring{A}})$$

$$\boxed{\frac{U_{tot}}{N}\Big|_{q=1} = -7.92eV}$$

$$\boxed{\frac{U_{tot}}{N}\Big|_{q=2} = -38.8eV}$$