

Worksheet Solution (Chapter 3 Crystal Binding)

Ans. 1: (c)

Solution: $U(R) = -\frac{A}{R^m} + \frac{B}{R^n}$

$$\frac{dU(R)}{dR} = 0 \Rightarrow \frac{mA}{R^{m+1}} - \frac{nB}{R^{n+1}} = 0 \Rightarrow R_e = \left(\frac{nB}{mA}\right)^{\frac{1}{n-m}}$$

$$\left(\frac{d^2U}{dR^2}\right)_{R=R_e} > 0 \text{ (For minima or stable)}$$

$$\Rightarrow \frac{-m(m+1)A}{R_e^{m+2}} + \frac{n(n+1)B}{R_e^{n+2}} > 0 \quad \Rightarrow n(n+1)BR_e^{m+2} - m(m+1)AR_e^{n+2} > 0$$

$$\Rightarrow n(n+1)BR_e^m > m(m+1)AR_e^n, \quad \Rightarrow n(n+1)B > m(m+1)AR_e^{n-m}$$

Now putting the values of R_e , Then $n(n+1)B > m(m+1)A \times \frac{nB}{mA}$

$$n+1 > m+1 \Rightarrow n > m$$

Ans. 2: (d)

Solution: $U(R) = -\frac{A}{R^m} + \frac{B}{R^n}$

$$\frac{dU(R)}{dR} = 0 \Rightarrow -A \frac{d}{dR} R^{-m} + B \frac{d}{dR} R^{-n} = 0$$

$$\Rightarrow -A(-m)R^{-m-1} + B(-n)R^{-n-1} = 0$$

$$mAR^{-m-1} - nBR^{-n-1} = 0 \Rightarrow mAR^{-m-1} = nBR^{-n-1}$$

$$\frac{R^{-m-1}}{R^{-n-1}} = \frac{nB}{mA} \Rightarrow R^{-m-1+n+1} = \frac{nB}{mA}, \quad \left(\frac{nB}{mA}\right) = R^{n-m} \Rightarrow R = \left(\frac{nB}{mA}\right)^{\frac{1}{n-m}}$$

Ans. 3: (a)

Solution: $U(R) = -\frac{\alpha}{R^4} + \frac{B}{R^{12}}$

$$\frac{dU(R)}{dR} = 0 \Rightarrow \frac{d}{dR}(-\alpha R^{-4}) + \frac{d}{dR}(BR^{-12}) = 0$$

$$-\alpha(-4)R^{-5} - 12\beta R^{-13} = 0 \Rightarrow 4\alpha R^{-5} = 12\beta R^{-13}$$

$$\alpha = 3\beta R^{-13+5} \Rightarrow \alpha = 3\beta R^{-8}$$

$$R^{-8} = \left(\frac{\alpha}{3\beta} \right) \Rightarrow R = \left(\frac{3\beta}{\alpha} \right)^{1/8}$$

Ans. 4: (d)

Solution: $U = \frac{A}{R^6} + \frac{\beta}{R^{12}}, R_e = 3A^0, U = 1.8eV$

$$\frac{dU}{dR} = 0 \Rightarrow \frac{6A}{R^7} = \frac{12B}{R^{13}} = 0 \Rightarrow 6A - \frac{12B}{R^6} = 0$$

$$B = \frac{A}{2} R_e^6 \Rightarrow U = -\frac{A}{R^6} + \frac{AR^6}{2R^{12}} = -\frac{A}{2R_e^6}$$

$$\Rightarrow 1.8eV = \frac{-A}{2 \times 3^6 \times 10^{-60}}$$

$$A = -1.8 \times 1.6 \times 10^{-19} \times 2 \times 3^6 \times 10^{-60} \text{ Jm}^6, \quad \Rightarrow A = -4.19 \times 10^{-76} \text{ Jm}^6$$

Ans. 5: (c)

Solution: $U = -\frac{A}{R^6} + \frac{B}{R^{12}}, R_e = 3A^0 = 3 \times 10^{-10} \text{ m}$

$$D = -U_e = 1.8eV = 1.8 \times 1.6 \times 10^{-19} \text{ J}, m = 6, n = 12$$

$$D = -U_e = \frac{A}{R_e^m} \left(1 - \frac{m}{n} \right) \Rightarrow U_e = \frac{A}{R_e^m} \left(\frac{m}{n} - 1 \right)$$

$$U_e = \frac{A}{R_e^6} \left(\frac{6}{12} - 1 \right) \Rightarrow A = -2U_e R_e^6$$

$$A = 2 \times 1.8 \times 1.6 \times 10^{-19} \times (3 \times 10^{-10})^6, \quad A = 4.19 \times 10^{-76} \text{ Jm}^6$$

further, at equilibrium separation, the net force is zero i.e.

$$F = -\left(\frac{dU}{dR} \right)_{R=R_e} = \frac{6A}{R^7} - \frac{12B}{R^{13}} = 0$$

$$B = \frac{A(R_e)^6}{2} = \frac{4.19 \times 10^{-76} \times (3 \times 10^{-10})^6}{2} = 1.53 \times 10^{-133} \text{ Jm}^{12}$$

Further $F(R) = -\frac{dU}{dR} = 0$ will be minimum or maximum when $\frac{dF}{dR} = 0$ and $R = R_c$ (Critical separation).

$$\text{Thus, } \left(\frac{dF}{dR} \right)_{R=R_c} = \left(\frac{d^2U}{dR^2} \right)_{R=R_c} = -\frac{42A}{R_c^8} + \frac{156B}{R_c^{14}} = 0$$

$$-42A + \frac{156B}{R_c^6} = 0 \Rightarrow 42A = \frac{156B}{R_c^6}$$

$$R_c^6 = \frac{156}{42} \frac{B}{A} \Rightarrow R_c^6 = \frac{13}{7} R_e^6 \Rightarrow R_c = \left(\frac{13}{7}\right)^{1/6} \times 3 \times 10^{-10}$$

$$R_c = 3.33 \times 10^{-10} \text{ m} = 3.33 \text{ \AA}$$

Ans. 6: (c)

Solution: $R_e = 3.56 \text{ \AA} = 3.56 \times 10^{-10} \text{ m}$, $n = 11.5$, $A = 1.76$

The potential energy per ion pair is given by

$$U_e = -\frac{Ae}{4\pi\epsilon_0 R_e} \left(1 - \frac{1}{n}\right) eV = -\frac{Ae^2}{4\pi\epsilon_0 R_e} \left(1 - \frac{1}{n}\right) J$$

$$U_e = \frac{-1.76 \times 1.6 \times 10^{-19} \times 9 \times 10^9}{3.56 \times 10^{-10}} \times \frac{10.5}{11.5} eV, \quad U_e = -6.50 eV$$

Ans. 7: (c)

Solution: Given: $r_{Li} = 0.60 \text{ \AA}$, $r_{Cl} = 1.81 \text{ \AA}$

As the ions touch each other, equilibrium separation between the two ions will be,

$$r_e = (0.60 + 1.81) \text{ \AA} = 2.41 \text{ \AA}$$

The attractive force between the two ions is coulombic,

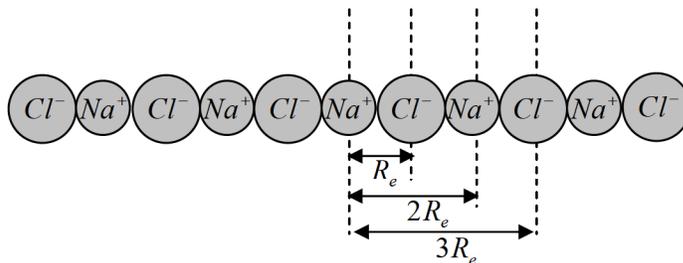
$$F = \frac{1}{4\pi\epsilon_0} \frac{q_1 q_2}{r_e^2}$$

$$F = \frac{9 \times 10^9 \times (1.6 \times 10^{-19})^2}{(2.41 \times 10^{-10})^2} = 3.96 \times 10^{-9} \text{ N}$$

Ans. 8: (b)

Solution: Madelung constant A is a function of crystal structure and can therefore be calculated from the geometrical arrangement of ions in a crystal.

To calculate the madelung constant for an infinite linear chain of ions of alternating charge, let us take one sodium ion as the reference ion and then write various terms of the series for alternating ions



$$A = 2 \left(\frac{1}{1} - \frac{1}{2} + \frac{1}{3} - \frac{1}{4} + \dots \right)$$

$$\left\{ \log_e(1+x) = x - \frac{x^2}{2} + \frac{x^3}{3} - \frac{x^4}{4} + \dots \right\}$$

$$A = 2 \log_e 2 \quad (\text{put } x=1 \text{ in above equation then } A=1.3863)$$

Ans. 9:

Solution: $U = -\frac{A}{R^m} + \frac{B}{R^n}$

$$U = -\frac{A}{R^2} + \frac{B}{R^{10}} \Rightarrow \frac{dU}{dR} = \frac{2A}{R^3} - \frac{10B}{R^{11}} = 0$$

$$2A = \frac{10B}{R^8} \Rightarrow A = \frac{5B}{R^8} \Rightarrow R_e^8 = \frac{5B}{A}$$

$$U = -\frac{A}{R^2} + \frac{B}{R^{10}} = \frac{1}{R_e^2} \left[\frac{B}{R^8} - A \right] = \frac{1}{R_e^2} \left[\frac{AB}{5B} - A \right]$$

$$U = \frac{1}{R_e^2} \left[\frac{A}{5} - A \right] = \frac{-1}{R_e^2} \left[\frac{4A}{5} \right] = -\frac{4}{5} \left[\frac{A}{R_e^2} \right]$$

Ans. 10: (b)

Solution: $R_e = 2.81A^0$, $A = 1.7476$ & $n = 9$

$$\text{Compressibility } (k_0) = \frac{72\pi\epsilon_0 R_e^4}{(n-1)Ae^2}$$

$$k_0 = \frac{18 \times 4\pi\epsilon_0 R_e^4}{(n-1)Ae^2} = \frac{18 \times (2.81 \times 10^{-10})^4}{9 \times 10^9 \times 8 \times 1.7476 \times e^2}$$

$$k_0 = \frac{18 \times (2.81)^4 \times 10^{-40}}{9 \times 10^9 \times 8 \times 1.7476 \times (1.6)^2 \times 10^{-38}}$$

$$k_0 = 3.48 \times 10^{-11} m^2 N$$