Assignment-3:-

Q-1:- Draw a diagram that depicts the variation of interatomic force as a function of spacing in terms of its attractive and repulsive components. Derive the expression for Equilibrium spacing.

Soln, The Equilibrium spacing will occur when the bond Energy (F_n) is minimum. This is when the net force between the two atoms is zero:-

$F_n = F_a + F_r = 0$

Where, F_a = attractive force

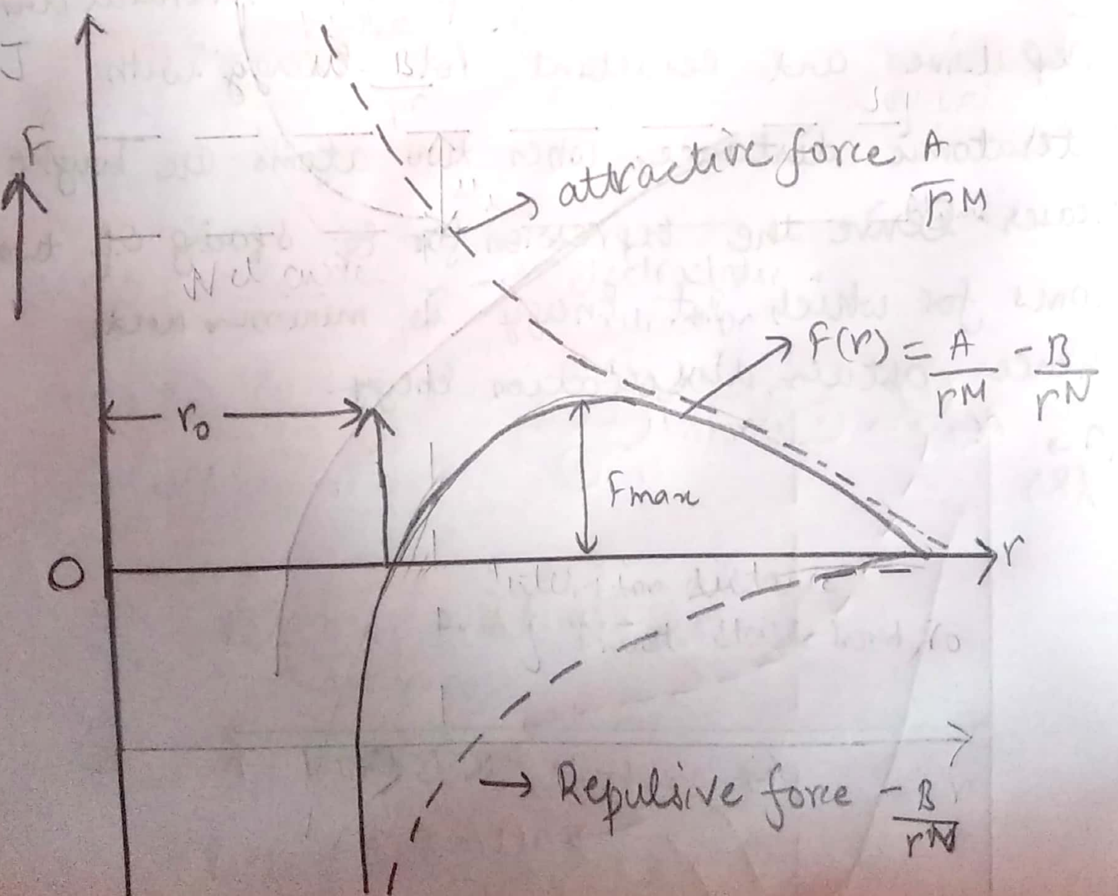
F_r = repulsive force.

The force between atoms is given as-

$$\boxed{F = \frac{du}{dr}}$$

where, u = bond energy

r = atomic separation



suppose two atoms exert attractive and repulsive forces on each other such that bonding force is-

$$F(r) = \frac{A}{r^M} - \frac{B}{r^N} \quad \text{where } N > M$$

$r \to$ centre to centre spacing b/n atoms

at Equillibrium when $r = r_0$

$F(r) = 0$

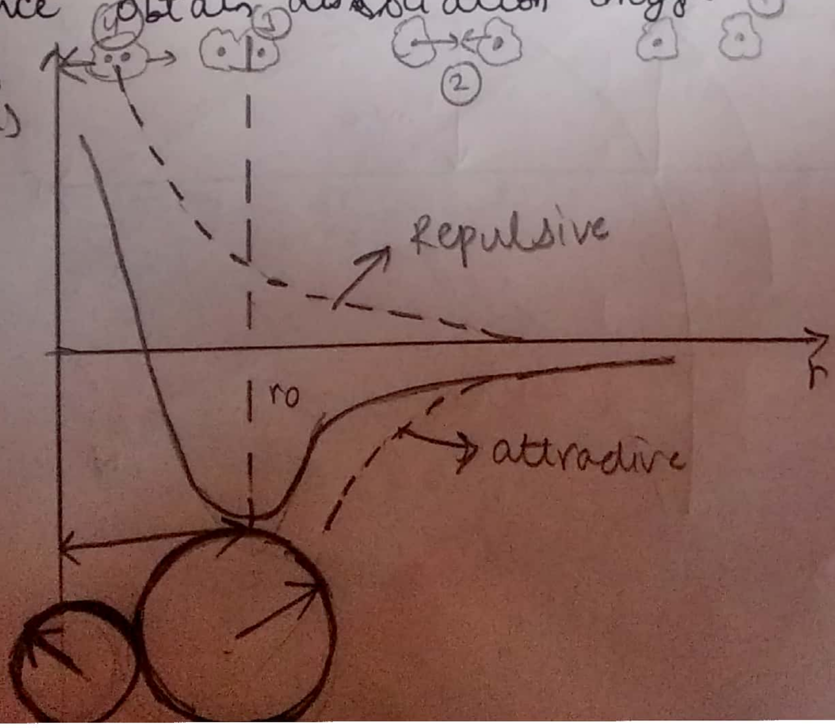
Thus, $\frac{A}{r^M} - \frac{B}{r^N} = 0$

$$\Rightarrow r_0^{N-M} = B/A$$

$$\Rightarrow \boxed{r_0 = (B/A)^{\frac{1}{N-M}}}$$

Q-2 → Plot the variation of attr. Potential and repulsive and resultant Pot. Energy with interatomic distance, when two atoms are bought nearer. Derive the expression for Eq. spacing of two atoms for which Pot Energy is minimum and hence obtain dissociation Energy

Soln →



$$U(r) = \frac{-a}{r^m} + \frac{b}{r^n}$$

at Equillibrium repulsive force becomes Equal to att. part

Let r_0 be the distance b/n the atoms for this min. $U(r)$ to occur

$U(r=r_0)_{min} \rightarrow$ -ve

$r_0 \rightarrow$ Eq. spacing of the system

$U(r)$ is min at $r=r_0$

$$\Rightarrow \left(\frac{du}{dr}\right)_{r=r_0} = 0$$

$$\Rightarrow \frac{ma}{r_0^{m+1}} - \frac{nb}{r_0^{n+1}} = 0$$

$$\Rightarrow \boxed{r_0 = \left(\frac{nb}{ma}\right)^{\frac{1}{n-m}}}$$

The Energy req. to dissociate the two atoms of molecule into an infinite separation. This is called Energy of dissociation.

$$U(r) = \frac{-a}{r^m} + \frac{b}{r^n}$$

$U(r)$ is min. at $r=r_0$

$$\Rightarrow U(r) = \frac{-a}{r_0^m} + \frac{b}{r_0^m} \quad (1)$$

$$\Rightarrow \left(\frac{du}{dr}\right)_{r=r_0} = 0$$

$$\Rightarrow r_0^n = r_0^m\left[\frac{bn}{am}\right]$$

Putting value of r_0^n in (1)

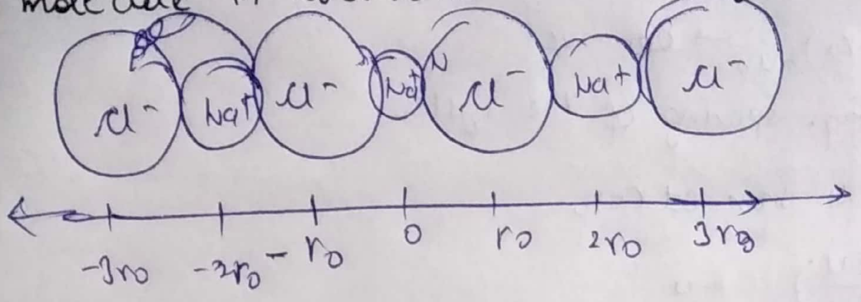
$$\Rightarrow U_{min} = \frac{-a}{r_0^m} + b\left[\frac{a}{b}\right]\left[\frac{m}{n}\right]\frac{1}{r_0^m}$$

$$= -\frac{a}{r_0^m}\left[\frac{m}{n} - 1\right]$$

$$\Rightarrow \boxed{U_{min} = \frac{-a}{r_0^m}\left[1 - \frac{m}{n}\right]}$$

Q-1 → Derive an Expression for lattice Energy in Ionic crystal and prove that madelung Const for molecule in NaCl like ionic crystal is 2ln2

Sol^n →



Attractive Coulomb Energy due to nearest neighbours-

$$\left[\frac{-e^2}{4\pi\varepsilon_0 r_0}\right] + \left[\frac{-e^2}{4\pi\varepsilon_0 r_0}\right] = \frac{-2e^2}{4\pi\varepsilon_0 r_0}$$

Repulsive Energy due to two +ve ions at dist. $2r_0$ is $= \frac{2e^2}{4\pi\varepsilon_0(2r_0)}$

attractive coloumb Energy due to next neighbours at a distance $3r_0$ is

$$\frac{-2e^2}{4\pi\varepsilon_0(3r_0)}$$

Thus, total energy due to all ions is

$$= \frac{-2e^2}{4\pi\varepsilon_0 r_0} + \frac{2e^2}{4\pi\varepsilon_0(2r_0)} - \frac{2e^2}{4\pi\varepsilon_0(3r_0)}$$

$$= -\frac{2e^2}{4\pi\varepsilon_0 r_0}\left[1 - \frac{1}{2} + \frac{1}{3} - \frac{1}{4} + - \right]$$

$$= \frac{-2e^2}{4\pi\varepsilon_0 r_0}\log(1+1)$$

$$= \frac{-e^2}{4\pi\varepsilon_0 r_0} 2\log 2$$

Now, 2 log 2 is Madelung Const. per molecule of ionic solid