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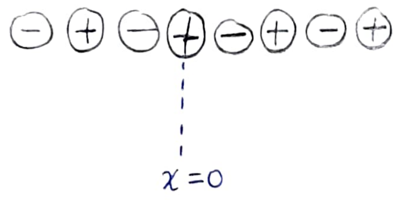
PHY1213 Tutorial Presentation

Madelung Constant for a 1D Crystal



Problem: Calculate the potential of a ion within a crystal due to all the other ions within the crystals (assume the ions to behave like point charges)

Potential Energy due to interaction with nearest neighbours $= \dfrac{-e^2}{4\pi\varepsilon_0 r_0} + \left(\dfrac{-e^2}{4\pi\varepsilon_0 r_0}\right)$

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

Next nearest neighbours (second shell) $= \dfrac{+e^2}{4\pi\varepsilon_0 (2r_0)} + \left(\dfrac{e^2}{4\pi\varepsilon_0 (2r_0)}\right)$

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

Next next nearest neighbours $= \dfrac{-e^2}{4\pi\varepsilon_0 (3r_0)} - \dfrac{e^2}{4\pi\varepsilon_0 (3r_0)}$

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

Thus the total energy due to all the ions in a linear array = E

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

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

Using expansion : $\ln(1+x) = x - \frac{x^2}{2} + \frac{x^3}{3} - \frac{x^4}{4} \ldots\ldots$

putting $x=1$ $\ln 2 = 1 - \frac{1}{2} + \frac{1}{3} - \frac{1}{4}$

$$W = E = \frac{-e^2}{4\pi\varepsilon_0 r_0} (2\ln 2)$$

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

Here α_m is called Madelung's constant

It is a property of a crystal which depends on various lattice parameters

The higher the α_m value, more is the PE interaction within a lattice, generally the crystal is more closely packed.