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Physics - 2 (15B11PH211)

Assignment - 5

Madelung Constant in 3D NaCl Crystal Structure.

The Coulomb energy of this Na^+ at A in the field of other ions is :

$$U = \frac{-6e^2}{4\pi\varepsilon_0 r_0} + \frac{12e^2}{4\pi\varepsilon_0(\sqrt{2}r_0)} - \frac{8e^2}{4\pi\varepsilon_0(\sqrt{3}r_0)} + \frac{6e^2}{4\pi\varepsilon_0(2r)} + \cdots$$

$$U = \frac{-e^2}{4\pi\varepsilon_0 r_0}\left[6 - \frac{12}{\sqrt{2}} + \frac{8}{\sqrt{3}} - \frac{6}{\sqrt{4}} + \cdots\right]$$

For mol of the Crystal, the total Coulomb energy is

$$U = \frac{-N_A e^2}{4\pi\varepsilon_0 r_0}\left[6 - \frac{12}{\sqrt{2}} + \frac{8}{\sqrt{3}} - \frac{6}{\sqrt{4}} + \cdots\right]$$

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

$A \rightarrow$ modelung constant & $A = 1.75$ for NaCl structure.