Tutorial Sheet-8 (Even Semester, 2022) - Physics-2(15B11PH211)

Assignment 5: Madelung constant in three dimensional NaCl crystal structure.

P1. The potential energy U(r) of a diatomic molecule is given by the expression, $U(r) = -\frac{a}{r^m} + \frac{b}{r^n}$, where, r is the inter-atomic distance, and "a" and "b" are constants. Derive the expression of equilibrium spacing of the atoms and dissociation energy. **[CO2]**

P2. The interaction energy of two particles in the field of each other is given by, $U(r) = -\frac{a}{r} + \frac{b}{r^9}$, where, r is the inter-atomic distance, and "a" and "b" are constants. Show that (i) particles form a stable compound for $r = r_0 = \left[\frac{9b}{a}\right]^{1/8}$; (ii) the ratio of the energy of attraction to the energy of repulsion is 9; (iii) the potential energy of the stable configuration is $-\left[\frac{a}{r_0}\right]\left[\frac{8}{9}\right]$. **[CO3]**

P3. The potential energy of a diatomic molecule is given by $U(r) = -\frac{a}{r^2} + \frac{b}{r^{10}}$, where, r is the inter-atomic distance. Estimate the equilibrium spacing of atoms and dissociation energy. Use $a=1.44\times10^{-39}$ Joule m^2, and $b=2.19\times10^{-115}$ Joule m^{10}. **[CO3]**

P4. What is Madelung constant? Show that for a 1-D array of ions of alternating sign with equal distance between two successive ions is $2Log2$. **[CO2]**

P5. Explain the terms, (i) ionization energy; (ii) lattice energy; (iii) cohesive energy; and (iv) electron affinity. **[CO1]**

P6. Estimate the binding energy (i.e. lattice energy) in eV/molecule of NaI for which the nearest neighbor distance is 0.324 nm. The Madelung constant for NaI = 1.748 and n= 9.5 **[CO3]**

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