

Condensed matter physics - 2017

Indian Institute of Science Education and Research Bhopal

Assignment 1

Atomic forces and bonding

1. The interaction energy of two particles in the field of each other is given by

$$U(r) = -\frac{\alpha}{r} + \frac{\beta}{r^9}, \quad \alpha \text{ and } \beta \text{ are constants.}$$

(i) Find out the distance between them for which they form a stable compound.

(iii) What is the configuration energy at equilibrium ?

(ii) What is the ration of attraction energy and repulsion energy at equilibrium ?

2. Instead of Born approximation for repulsive energy, consider Born-Mayer model for repulsive part of the potential

$$U_{ij}^{\text{repul}} = \lambda_{ij} \exp\left(-\frac{|\vec{r}_{ij}|}{\rho}\right)$$

where, λ_{ij} and ρ are empirical constant parameters. Consider nearest neighbor repulsions, for which $\lambda_{ij} = \lambda$. Also consider there are z number of nearest neighbours. Calculate average energy of a single ion in presence of other ions. Estimate the value of ρ from the data given in class.

3. Suppose an atom A has ionization energy 6 eV and atom B has electron affinity of 4 eV . Inter-atomic distance is 0.3 nm . Find bond energy. Consider monovalent ionic bond.

4. Calculate Madelung constant of a square lattice of side a . $+q$ and $-q$ charges are sitting alternatively at each site.