2.10 *The net potential energy between two adjacent ions, E_N, may be represented by the sum of Equations 2.9 and 2.11; that is,*

$$E_N = -\frac{A}{r} + \frac{B}{r^n} \tag{2.17}$$

Calculate the bonding energy E_0 in terms of the parameters A, B, and n using the following procedure:

1. Differentiate E_N with respect to r, and then set the resulting expression equal to zero, because the curve of E_N versus r is a minimum at E_0.

2. Solve for r in terms of A, B, and n, which yields r_0, the equilibrium interionic spacing.

3. Determine the expression for E_0 by substitution of r_0 into Equation 2.17.

Solution

(a) Differentiation of Equation 2.17 yields

$$\frac{dE_N}{dr} = \frac{d\left(-\frac{A}{r}\right)}{dr} + \frac{d\left(\frac{B}{r^n}\right)}{dr}$$

$$= \frac{A}{r^{(1+1)}} - \frac{nB}{r^{(n+1)}} = 0$$

(b) Now, solving for r (= r_0)

$$\frac{A}{r_0^2} = \frac{nB}{r_0^{(n+1)}}$$

or

$$r_0 = \left(\frac{A}{nB}\right)^{1/(1-n)}$$

(c) Substitution for r_0 into Equation 2.17 and solving for E (= E_0) yields

$$E_0 = -\frac{A}{r_0} + \frac{B}{r_0^n}$$

$$= -\frac{A}{\left(\frac{A}{nB}\right)^{1/(1-n)}} + \frac{B}{\left(\frac{A}{nB}\right)^{n/(1-n)}}$$

2.11 *For a Na^+–Cl^- ion pair, attractive and repulsive energies E_A and E_R, respectively, depend on the distance between the ions r, according to*

$$E_A = -\frac{1.436}{r}$$

$$E_R = \frac{7.32 \times 10^{-6}}{r^8}$$

For these expressions, energies are expressed in electron volts per Na^+–Cl^- pair, and r is the distance in nanometers. The net energy E_N is just the sum of the preceding two expressions.

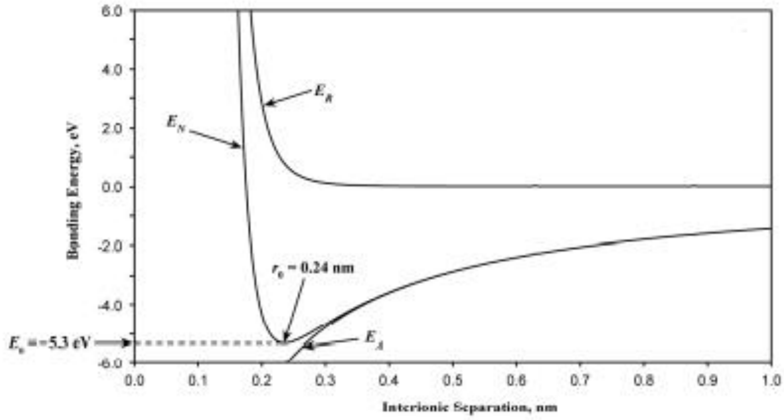
(a) Superimpose on a single plot E_N, E_R, and E_A versus r up to 1.0 nm.

(b) On the basis of this plot, determine (i) the equilibrium spacing r_0 between the Na^+ and Cl^- ions, and (ii) the magnitude of the bonding energy E_0 between the two ions.

(c) Mathematically determine the r_0 and E_0 values using the solutions to Problem 2.10, and compare these with the graphical results from part (b).

Solution

(a) Curves of E_A, E_R, and E_N are shown on the plot below.



(b) From this plot:

$r_0 = 0.24$ nm

$E_0 = -5.3$ eV

(c) From Equation 2.17 for E_N

$$A = 1.436$$
$$B = 7.32 \times 10^{-6}$$
$$n = 8$$

Thus,

$$r_0 = \left(\frac{A}{nB}\right)^{1/(1-n)}$$

$$= \left[\frac{1.436}{(8)(7.32 \times 10^{-6})}\right]^{1/(1-8)} = 0.236 \text{ nm}$$

and

$$E_0 = -\frac{1.436}{\left[\frac{1.436}{(8)(7.32 \times 10^{-6})}\right]^{1/(1-8)}} + \frac{7.32 \times 10^{-6}}{\left[\frac{1.436}{(8)(7.32 \times 10^{-6})}\right]^{8/(1-8)}}$$

$$= -5.32 \text{ eV}$$

Mixed Bonding

2.14 *(a) Calculate %IC of the interatomic bonds for the intermetallic compound Al_6Mn. (b) On the basis of this result what type of interatomic bonding would you expect to be found in Al_6Mn?*

Solution

(a) The percent ionic character is a function of the electron negativities of the ions X_A and X_B according to Equation 2.16. The electronegativities for Al and Mn (Figure 2.9) are 1.5 and 1.6, respectively. Therefore, the percent ionic character is determined using Equation 2.16 as follows:

$$\%\text{IC} = \left[1 - \exp(-0.25)(1.6-1.5)^2\right] \times 100 = 0.25\%$$

(b) Because the percent ionic character is exceedingly small (0.25%) and this intermetallic compound is composed of two metals, the bonding is completely metallic.

Secondary Bonding or van der Waals Bonding

2.13 *Explain why hydrogen fluoride (HF) has a higher boiling temperature than hydrogen chloride (HCl) (19.4 vs. –85°C), even though HF has a lower molecular weight.*

Solution

The intermolecular bonding for HF is hydrogen, whereas for HCl, the intermolecular bonding is van der Waals. Since the hydrogen bond is stronger than van der Waals, HF will have a higher melting temperature.

Bonding Type-Material Classification Correlations

2.15 *What type(s) of bonding would be expected for each of the following materials: solid xenon, calcium fluoride (CaF_2), bronze, cadmium telluride (CdTe), rubber, and tungsten?*

Solution

For solid xenon, the bonding is van der Waals since xenon is an inert gas.

For CaF_2, the bonding is predominantly ionic (but with some slight covalent character) on the basis of the relative positions of Ca and F in the periodic table.

For bronze, the bonding is metallic since it is a metal alloy (composed of copper and tin).

For CdTe, the bonding is predominantly covalent (with some slight ionic character) on the basis of the relative positions of Cd and Te in the periodic table.

For rubber, the bonding is covalent with some van der Waals. (Rubber is composed primarily of carbon and hydrogen atoms.)

For tungsten, the bonding is metallic since it is a metallic element from the periodic table.