HW#1 due September 20

1. The net potential energy between two adjacent ions, EN, may be represented by the sum of equations for attractive energy and repulsive energyand 

that is,

Calculate the bonding energy *E0* in terms of the parameters *A*, *B*, and *n* using the following procedure:

(1) Differentiate *EN* with respect to *r*, and then set the resulting expression equal to zero, since the curve of *EN* versus *r* is a minimum at *E0*.

(2) Solve for *r* in terms of *A*, *B*, and *n*, which yields *r0*, the equilibrium interionic spacing.

(3) Determine the expression for *E0* by substitution of *r0* into Equation,.

2. For a Na+–Cl– ion pair, attractive and repulsive energies *EA* and *ER*, respectively, depend on the distance between the ions *r*, according to

, 

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

(a) Superimpose on a single plot *EN*, *ER*, and *EA* versus *r* up to 1.0 nm.

(b) On the basis of this plot, determine (i) the equilibrium spacing *r0* between the Na+ and Cl– ions, and (ii) the magnitude of the bonding energy *E0* between the two ions.

(c) Mathematically determine the *r0* and *E0* values using the solutions to #1, and compare these with the graphical results from part (b).

3. (a) Calculate %IC (ionic character) of the interatomic bonds for the intermetallic compound Al6Mn. The electronegativities for Al and Mn are 1.5 and 1.6, respectively.

(b) On the basis of this result what type of interatomic bonding would you expect to be found in Al6Mn?

4. 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.

5. What type(s) of bonding would be expected for each of the following materials: solid xenon, calcium fluoride (CaF2), bronze, cadmium telluride (CdTe), rubber, and tungsten?