ASSIGNMENT 2

Reading: Kittel, Chapters 3, 1

Problems

1. Classify the types of bonding in the following solids according to: covalent, ionic, metallic, van der Waals, etc. Briefly explain your reasoning.

(a) KI (b) SiO_2 (c) Ca (d) GaAs (e) Xe (f) C (diamond) (g) C (graphite) (h) H_2O (ice)

2. Consider a solid composed of N atoms interacting via the potential:

$$U(r) = \frac{A}{r^{12}} - \frac{B}{r^6}$$

(a) Assuming only nearest neighbor interactions, calculate the equilibrium lattice spacing.

(b) Calculate the binding energy of the solid if each atom has 8 nearest neighbors. (N.B. Be sure to count nearest neighbor *pairs* only.)

3. Consider the sp^2 hybrid wavefunction (for example, graphitic carbon)

$$\phi = as + bp_x + cp_y.$$

Find values of a, b, and c such that the (3) wavefunctions are normalized and mutually orthogonal with positive lobes at 120 deg with respect to each other in the x-y plane.

4. If atoms are considered as contacting hard spheres show that:

(a) the bcc lattice has packing fraction 0.68

(b) the fcc lattice has packing fraction 0.74

(c) the hcp structure has c/a = 1.633

(d) for a cube of side a, what is the "atomic diameter" in the bcc and fcc cases?

5. Given a bcc structure formed by hard spheres, what is the largest sphere that can be introduced, not at a lattice site, without distorting the initial bcc arrangement? Where would these extra spheres be placed? These locations are called *interstitial* sites.

Be sure to show calculations and geometrical sketches in 4 and 5.