

MS 115a, Problem Set #1

assigned 10/03/12

due 10/10/12

**Reading:** Tilley: Chap. 1, excluding section 1.4; Shackelford: Chap. 2, content on coordination number will be covered in the following week (can skip for now).

- Sodium chloride (NaCl) and cesium iodide (CsI) exhibit predominantly ionic bonding. The  $\text{Na}^+$ ,  $\text{Cl}^-$ ,  $\text{Cs}^+$  and  $\text{I}^-$  ions have electron structures that are identical to which inert gases?
- Determine, for each of the electron configurations given below, whether the element is an inert gas, a halogen, an alkali metal, an alkaline earth metal, or a transition metal. Justify your choices.
  - $1s^2 2s^2 2p^6 3s^2 3p^6 3d^7 4s^2$
  - $1s^2 2s^2 2p^6 3s^2 3p^6$
  - $1s^2 2s^2 2p^5$
  - $1s^2 2s^2 2p^6 3s^1$
  - $1s^2 2s^2 2p^6 3s^2 3p^6 3d^2 4s^2$
  - $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$
- Each electron has a distinct set of four quantum numbers. Indicate the set of quantum numbers of each of the valence electrons in aluminum (Al), magnesium (Mg), iron (Fe), titanium (Ti), chromium (Cr), bismuth (Bi) and tellurium (Te).
- Assuming purely electrostatic interactions, calculate the force of attraction between a  $\text{Ca}^{2+}$  and an  $\text{O}^{2-}$  ion, the centers of which are separation by a distance of 0.43 nm.
- The net potential energy between two adjacent ions,  $E_N$ , may be represented by the expression,

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

where  $r$  is the interionic separation and  $A$ ,  $B$  and  $n$  are constants, and where the first term in the expression reflects the long-range attractive interaction and the second term the short-range repulsive interaction.

- Derive an expression for  $r_o$ , the equilibrium interionic separation in terms of the material parameters  $A$ ,  $B$ , and  $n$ .
  - Derive the value of the bonding energy  $E_o$  [ $= E_N(r_o)$ ] in terms of the same parameters  $A$ ,  $B$ , and  $n$ .
- Consider two hypothetical metals D and J. For both these metals, the potential well describing the bonding can be written in the form given in problem 5. For metal D, the parameters  $A$ ,  $B$  and  $n$  are given by 10, 12 and 8, respectively, where the energy,

$E$ , is measured in eV, and the interatomic separation,  $r$ , in Å. For metal J, the parameters are 5, 7 and 6. Determine which has the higher

- (a) interatomic distance
- (b) melting temperature
- (c) thermal expansion coefficient

(d) Young's modulus [ $\sim$  proportional to  $\left. \frac{\partial^2 E_N}{\partial r^2} \right)_{r=r_0}$  ]

7. What type(s) of bonding would be expected for each of the following materials: brass (a copper-zinc alloy), rubber, barium sulfide (BaS), solid xenon, bronze (a copper-tin alloy), nylon, and aluminum phosphide (AlP)?
8. We have described metallic bonding in terms of charged ion cores and a sea or gas of free electrons. Determine the number density of free electrons in gold, assuming each atom contributes one electron to the 'electron gas.' The molar mass of gold is  $0.19697 \text{ kg mol}^{-1}$  and the density is  $19281 \text{ kg m}^{-3}$ .
9. Briefly cite the main differences between ionic, covalent and metallic bonding.
10. Offer an explanation as to why covalently bonded materials are generally less dense than ionically or metallically bonded ones.
11. The atomic packing factor for a crystal structure is defined as the ratio of volume occupied by the atoms in the unit cell to the total volume of the unit cell. Show that the atomic packing factor
  - (a) for the cubic close-packed (CCP) structure is 0.74
  - (b) for the ideal hexagonal close-packed (HCP) structure is 0.74
  - (c) for the body-centered cubic packed structure is 0.68