HW 2	Inorganic Materials Chemistry	Name:	
Points:	**C7780**	**Date:**	
Max. 100 points	**Fall 2016**	**A**	

1. (10 pts) Copper metal crystallizes with a cubic close packed (ccp or fcc) structure having a lattice parameter a = 3.6147 Å. Calculate the Cu-Cu distance (separation) between nearest-neighbor Cu atoms in the crystal. **Hint:** nearest-neighbor Cu atoms are any two within the same close-packed layer (plane).

2. (10 pts) Molybdenum metal crystallizes with a body-centered cubic (bcc) structure having a lattice parameter a = 3.1469 Å. Calculate the Mo-Mo distance (separation) between nearest-neighbor Mo atoms in the crystal. **Hint:** the nearest-neighbor atoms are aligned along the body diagonal of the bcc unit cell.

3. (10 pts) The compound AgCl exhibits the NaCl structure. Frenkel defects in AgCl result from placement of Ag^+ ions in T sites of the Cl^- sublattice. These displaced Ag^+ ions are associated with Ag^+ vacancies elsewhere in the crystal. Sketch a diagram of the AgCl structure that clearly depicts the environment around a Ag^+ ion in a T defect site. Describe the number and nature of cation and anion nearest neighbors about the interstitial Ag^+ ion. What characteristic or characteristics of the compound or crystal structure may stabilize such a defect?

4. (35 pts) Use the Born-Landé equation (use UPDATED presentation in IS) and the appropriate Shannon-Prewitt radii (provided below) to calculate lattice energies (L_0) for the following structures. Comment on results.
a. CsCl having the CsCl structure: r_{Cs+}(CN8) = 1.88 Å; r_{Cl-}(CN6) = 1.67 Å (CN8 not avail.)
b. CsCl having the NaCl structure: r_{Cs+}(CN6) = 1.81 Å; r_{Cl-}(CN6) = 1.67 Å
c. NaCl having the NaCl structure: r_{Na+}(CN6) = 1.16 Å; r_{Cl-}(CN6) = 1.67 Å
d. NaCl having the CsCl structure: r_{Na+}(CN8) = 1.32 Å; r_{Cl-}(CN6) = 1.67 Å (CN8 not avail.)
e. ZnS having the sfalerite structure: r_{Zn2+}(CN4) = 0.74 Å; r_{S2-}(CN6) = 1.70 Å (CN4 not avail.)
f. ZnS having the wurtzite structure: r_{Zn2+}(CN4) = 0.74 Å; r_{S2-}(CN6) = 1.70 Å (CN4 not avail.)
g. ZnS having the NaCl structure: r_{Zn2+}(CN6) = 0.88 Å; r_{S2-}(CN6) = 1.70 Å

5. (15 pts) Consider the direct reaction of polycrystalline Fe_2O_3 and TiO_2 to form $FeTiO_3$.
a) Write a balanced equation for the reaction.
b) Calculate the quantity of each starting reagent necessary to produce 2.500 g of product.
c) At what temperature would you carry out the reaction?

d) If all of the TiO_2 and Fe_2O_3 particles were cubes, 10 μm on an edge, how many crystallites of each reagent would there be? (Hint: You may need to consult a primary source, e.g. CRC handbook, to obtain the density and melting points of the reactants)

6. (20 pts) Assume that CaO reacts with CeO_2 and forms $CaCeO_3$.
a) What could be the structure type of this compound? _______________
b) Write balanced chemical equations for the reactions taking place at the interfaces (assume counter diffusion of both cations) and calculate the Kirkendall ratio for this process.

I **II**

CaO	**$CaCeO_3$**	**CeO_2**