HW 2	**Inorganic Materials Chemistry**	Name:	
Points:	**C7780**	**Date:**	
Max. 100 points	**Fall 2019**	**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. (20 pts) Derive the first three terms of the series to calculate the Madelung constant for CsCl. Use interionic separation d ($d = r_{Cs^+} + r_{Cl^-}$) as the distance parameter in the Coulomb equation.

Cl⁻
Cs⁺

CsCl
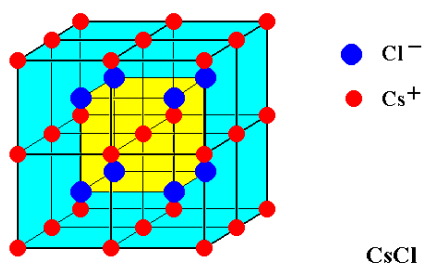
4. (10 pts) Should it be possible to convert β-cristobalite to some of the other modifications by applying high pressure?

Modification of SiO_2	Density / g cm^{-1}
α-quartz	2.65
β-quartz	2.53
β-tridymite	2.27
β-cristobalite	2.33
Vitreous	2.20

5. (15 pts) a) Write balanced chemical equation for a solid state reaction:

$$ZnC_2O_4 + \quad Fe(OH)_3 \rightarrow \quad ZnFe_2O_4$$

b) What is the driving force in this reaction?

c) Cubic spinel $ZnFe_2O_4$ crystallizes with 8 formula units in the cubic unit cell. The cell parameter $a = 8.42$ Å. Calculate the density in g cm^{-3} of the material.
$N_A = 6.022141 \cdot 10^{23}$ mol^{-1}, $A_r(Zn) = 65.41$, $A_r(Fe) = 55.85$, $A_r(O) = 15.999$.

6. (15 pts) The cell parameter for cubic spinel $ZnFe_2O_4$ is $a = 8.42$ Å, for $MnFe_2O_4$ $a = 8.50$ Å.
a) Suggest a reason for the difference.

b) What would be the cell parameter for the mixed-metal phase $(Mn_xZn_{1-x})Fe_2O_4$ when x = 0.25, 0.50, and 0.75.

7. (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 interface **I** and **II** (assume counter diffusion of both cations) and calculate the Kirkendall ratio for this process.

	I		**II**	
	CaO	**CaCeO₃**	**CeO₂**	