Solid State Modeling Worksheet

As you work through the steps in the lab procedures, record your experimental values and the results on this worksheet.

Question A1: Looking from above, how much of the atom is inside the shaded region?

Question A2: The corner of a cubic unit cell such as this one is *defined by the center (nucleus) of the atom at the corner.* How much of this atom is above the nucleus **and** inside the shaded region (inside the unit cell)?

Question A3: How many total atoms are inside the unit cell (defined by the centers of the eight spheres)?

Question A4: Using a ruler, measure the length of a side of your unit cell in cm. (Remember, the unit cell is defined by the nuclei of the atoms!) What is the volume of your unit cell?

Question A5: We will define "atom density" for our unit cells as the number of spheres that can pack into a cubic centimeter. What is the "atom density" (spheres/cm^3) for your simple cubic cell?

Question A6: Noting as before that the corner of the unit cell is defined by the nucleus of this atom, how much of this atom is inside the unit cell?

Question A7: Focus on the layer 2 atom. How much of this atom is inside the unit cell?

Question A8: How many total atoms are inside the unit cell?

Question A9: Using a ruler, measure the length of a side for this unit cell. What is the volume (in cm^3) of this unit cell?

Question A10: What is the "atom density" (spheres/cm^3) for your body centered cubic cell?

Question A11:

a. Comparing this structure (body centered cubic) to the last structure (simple cubic), which one *appears* to have less void volume?

b. Compare your observation to your calculated "atom densities" for these two structures. Do your calculations confirm your observation?

Question A12: Focus on a layer 2 atom. How much of this atom is inside the unit cell?

Question A13: How many total atoms are inside the unit cell?

Question A14: Using a ruler, measure the length of a side of this unit cell. What is the volume (in cm^3) of this unit cell?

Question A15: What is the "atom density" (in spheres/cm^3) for your face centered cell?

Question A16:

a. Comparing this structure (face centered cubic) to the last structure (body centered cubic), which one *appears* to have less void volume?

b. Compare your observation to your calculated "atom densities" for these two structures. Do your calculations confirm your observation?

Question A17: Comparing the "atom densities" of all three cubic unit cells, rank them in packing efficiency, with the most efficiently packed cell listed first.

Question B1: Focus on *only* the colorless spheres. What type of cubic structure do they appear to be arranged in?

Question B2: Focus on *only* the blue spheres. What type of cubic structure do they appear to be arranged in? (You may need to build another set of layers 2 and 2 to see this.)

Question B3:

a. How many colorless spheres are inside the unit cell?

b. How many blue spheres are inside the unit cell?

c. What is the ratio of colorless to blue spheres in the unit cell?

d. What is the chemical formula for sodium chloride?

e. Do your results in part c reflect the correct stoichiometry in sodium chloride?

f. Based on your knowledge of trends in ionic radii, which spheres represent sodium ions and which represent chloride ions?

Question B4:

a. Focus on the central, colorless sphere of layer 1'. How many blue spheres are in contact with it? (You may need to build another set of layers 2 and 2 to see this.) This is its coordination number.

b. Focus on the central, blue sphere of layer 2. How many colorless spheres are in contact with it?

Question B5: Focus on *only* the colorless spheres. What type of cubic structure do they appear to be arranged in?

Question B6:

a. How many colorless spheres are inside the unit cell?

b. How many green spheres are inside the unit cell?

c. What is the ratio of colorless to green spheres in the unit cell?

d. What is the chemical formula for cesium chloride?

e. Do your results in part c reflect the correct stoichiometry in cesium chloride?

f. Based on your knowledge of trends in ionic radii, which spheres represent cesium ions and which represent chloride ions?

Question B7: Focus only on the cube made by the 8 green spheres.

a. What type of cubic structure do the green spheres appear to be arranged in?

b. What is the ratio of colorless to green spheres?

Question B8: Using a ruler, compare the length of the side of a cube with colorless spheres on the corners to one with green spheres.

a. Do they have the same volume?

b. Are these both acceptable unit cells for cesium chloride? Why or why not?

Question B9:

a. Focus on one of the green spheres in layer 2. How many colorless spheres are in contact with it?

b. Focus on the colorless sphere at the center of the green cornered cube. How many green spheres are in contact with it?

Question B10:

a. Focus on *only* the colorless spheres. What type of cubic structure do they appear to be arranged in?

b. Focus on *only* the green spheres. What type of cubic structure do they appear to be arranged in?

Question B11: Putting the two ions together in this arrangement gives the "fluorite" structure. The name is derived from the mineral fluorite, which contains calcium fluoride.

a. How many colorless spheres are inside the unit cell?

b. How many green spheres are inside the unit cell?

c. What is the ratio of colorless to green spheres in a unit cell?

d. What is the chemical formula of calcium fluoride?

e. Do your results in part c reflect the correct stoichiometry in calcium fluoride?

f. Which spheres represent calcium ions and which represent fluoride ions?