**Developing methodology to evaluate nanotoxicology: Measuring density of nanoparticle aggregates.**

**THE PLAN:** We are going to investigate the relationship between the crystalline structure and physical properties by looking at density of materials. We will relate this to a real world example of nanotoxicology.

**WHY?** After spending all that time understanding crystalline solids, let’s put it to use in a real world situation!

**THE SCRIBE’S SHEET**

**THE SCRIBE’S SHEET (ONE PER GROUP)**

 **Name Role**

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ Scribe

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ Facilitator

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ Timekeeper

**NANOTOXICOLOGY (45 minutes)**

One of the major issues that comes up when studying the impact of nanomaterials on human health is a simple one: how do we accurately determine how many nanoparticles have made it into the cell? This is the question presented by DeLoid et al, 2014, *Nature Communications* (<https://doi.org/10.1038/ncomms4514>).

1. What is the major technical problem addressed in this paper?
2. What novel methodology are the authors using to look at this problem?
3. We are going to evaluate the effectiveness of their methods by comparing calculated and experimentally determined densities for several nanomaterials. First we are going to work with their standard: Au. Let’s calculate the density…Density is mass over volume. So let’s first calculate volume.
4. Gold crystallizes in the FCC unit cell. Draw the 2D projection below:

(0,1)

1. As opposed to the 2D projection above, draw a second projection showing a space filling model and indicate where the atoms are touching on just one face of the cube.
2. Look up the metallic radii for gold and write it below
3. Explain how you can use this information to calculate the length of cube (*a*) and provide the *a* length.
4. Now that you have the length in pm, convert to cm. Show your work.
5. Calculate the volume of the cube in cm3. Show your work.
6. Now we need to know mass. Look up the molar mass of gold and write it below. Be sure to write down the units.
7. Molar mass is in units of g/mol, but how many atoms do we have per unit cell?
8. Provide the mass within the unit cell.
9. Calculate the density of gold in g/cm3.
10. We will now choose two other materials to compare their experimental results to the actual densities. The first one is CeO2
11. First look up the uses of CeO2 nanoparticles online and explain its importance.
12. CeO2 crystallizes in the Fluorite structure. Draw the 2D projection below.

(0,1)

1. In this case the Ce atoms are not touching along the face of the cell, so we are going to use the unit cell length (5.43 Å) to calculate the volume in cm3. Calculate the volume of the CeO2 unit cell using the length.
2. Calculate the molar mass of CeO2
3. Calculate the mass of the atoms in the unit cell.
4. Calculate the density of CeO2
5. Next we will examine ZnO. ZnO crystallizes in the wurtzite and sphalerite structures. Calculate the density of ZnO for the sphalerite (Cubic cell with unit cell length = 4.62 Å) and wurtzite (hexagonal closest packing with a = 3.25 and c = 5.20 Å) structures. The 2D projection of the wurtizite structure is provided below for reference.

3/8

7/8

(1/2)

(0,1)

1. Now compare your work to the chart found in the paper. You will want to look at Table 1, particularly the columns labeled ρ ENM, ρEV, and ρ (NOTE: There is a mistake in Table 1. The column ρ actually corresponds to ρ ES in the footnotes). Provide a short description of each of the columns in the table.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Sample | Calculated Density (g/cm-3) | ρ ENM (g/cm-3) | ρ EV (g/cm-3) | ρ ES (g/cm-3) |
|  |  |  |  |  |
|  |  |  |  |  |
|  |  |  |  |  |
|  |  |  |  |  |

1. Are there any discrepancies in the calculated vs. experimental data? Can you explain those discrepancies?