Homework of VESTA software

1. **Magnesium oxide (MgO) structure.** The MgO lattice is face-centered cubic consisting of Mg^{2+} and O^{2-} by ionic bonding. It has similar structure to NaCl. (a) With 4 Mg and 4 O atoms in a unit cell, what values of the lattice parameters are required to set ($a = b = c =$? and $\alpha = \beta = \gamma =$?)? (b) Show the factional position values of the 8 atoms. (c) Draw the structure as figure 1.
2. **Cesium chloride (CsCl) structure.** The CsCl lattice is body-centered cubic. (a) With only two atoms in a unit cell, what values of the lattice parameters are required to set ($a = b = c =$? and $\alpha = \beta = \gamma =$?)? (b) Show the factional position values of the two atoms. (c) Draw the structure as figure 2.
3. **Cubic zinc sulfide (ZnS) structure.** The cubic ZnS structure, which is similar to the diamond structure, results when Zn atoms are placed on one fcc lattice and S atoms on the other fcc lattice. (a) With 4 Zn and 4 S atoms in a unit cell, what values of the lattice parameters are required to set ($a = b = c =$? and $\alpha = \beta = \gamma =$?)? (b) Show the factional position values of the 8 atoms. (c) Draw the structure as figure 3.

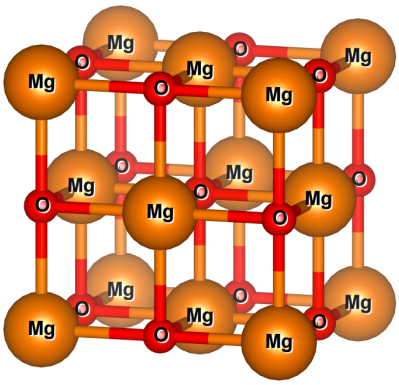


Figure 1

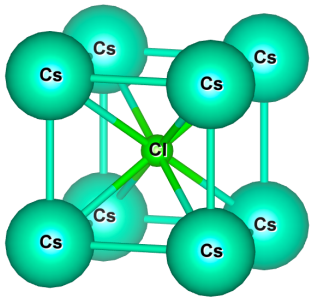


Figure 2

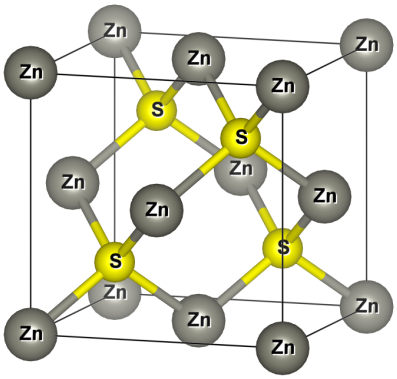


Figure 3

4. **Hexagonal close-packed cobalt (Co) structure.** The metallic cobalt below 450 °C is hexagonal close-packed. (a) With only two atoms in a unit cell, what values of the lattice parameters are required to set ($a = b = c$ =? and $\alpha = \beta = \gamma$ =?)? Hint: Find from the Table 3 in Kittel's book. (b) Show the factional position values of the two atoms. (c) Draw the structure as figure 4.1. (d) Repeat the unit cell over x and y direction and draw as figure 4.2.

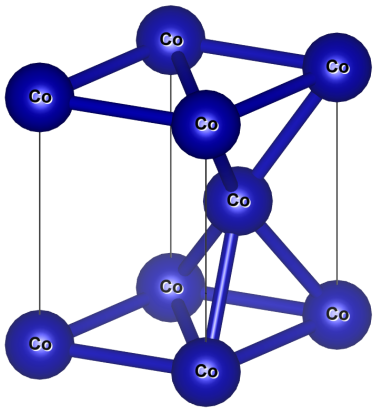


Figure 4.1

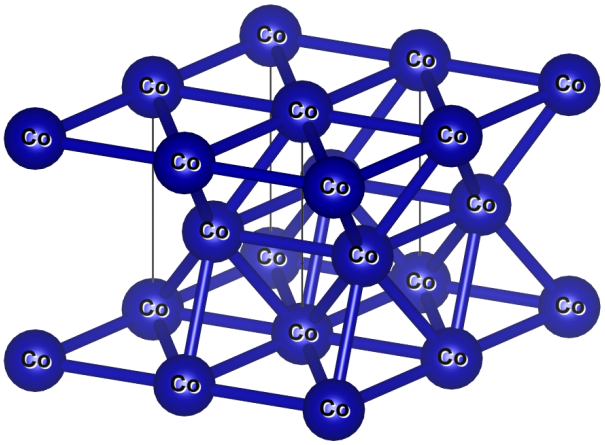


Figure 4.2

5. **Primitive sodium chloride (NaCl) structure.** In the class, TA showed an example of NaCl, which is an fcc lattice with 8 atoms in a cubic unit cell. From your textbook, primitive cell of fcc structure is rhombohedron. (a) With only two atoms in a unit cell, what values of the lattice parameters are required to set ($a = b = c$ =? and $\alpha = \beta = \gamma$ =?)? (b) Show the factional position values of the two atoms. (c) Draw the structure as figure 5. (d) Measuring the length of the following red line in VESTA, make sure it is equal to 5.63 Å.

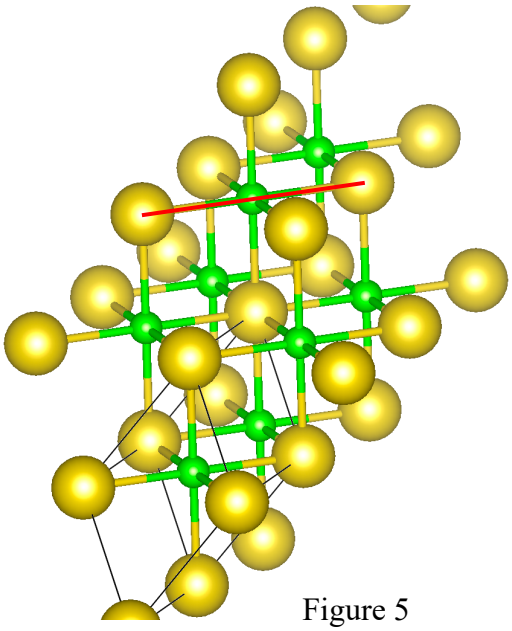
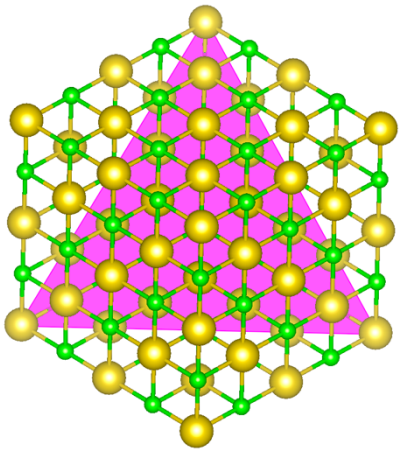
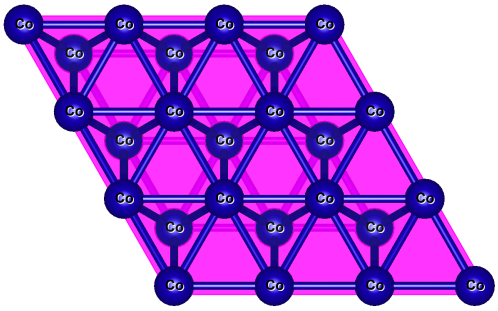


Figure 5

6. (a) Draw a (111) lattice plane of the NaCl, and (0001) lattice plane of hcp Co. (b) List three points that describe the difference or similarity between these structures.





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