**Literature Discussion of “A stable compound of helium and sodium at high pressure”**

Before class, read the following article:

Dong, X.; Oganov, A. R.; Goncharov, A. F.; Stavrou, E.; Lobanov, S.; Saleh, G.; Qian, G.-R.; Zhu, Q.; Gatti, C.; Deringer, V. L.; et al. A stable compound of helium and sodium at high pressure. *Nature Chemistry* **2017**, *9* (5), 440–445 DOI: 10.1038/nchem.2716.

**A. Comprehensive questions**

1. What were the goals of this project?
2. What specifically did the researchers do?  What specific methods were employed?
3. Why was the diamond anvil cell used? What properties made it particularly suitable for this experiment?
4. What was the major synthetic result of the paper?
5. The compound made in this paper is an electride. What is an electride?

**B. Atomic and molecular properties**

1. What are the properties of sodium at normal pressure? What is the unit cell? How do these change with increasing pressure? How do these change at very high pressure?

1. Why have compounds with helium not been observed? Why are compounds with xenon more readily observed?

1. What is an inclusion compound? What evidence do the authors give to support that this is not an inclusion compound?
2. Only Na is found to make these compounds with He at high pressures. How does sodium differ from the heavier alkali metals?

**C. Solid-state structure**

1. Describe the face-centered cubic (fcc) unit cell. How many atoms/ions are in lattice positions? Identify the type, number and location of the holes. (Note: the paper uses void as a synonym for hole)
2. Consider the unit cell for the sodium helium compound in the paper. Describe the occupancy, both location and contents, of the unit cell. Based on fractional unit cell counts, what is the formula for the sodium helium compound?
3. Fill in the interstitial electrons (or electrides) in the depiction of the unit cell in Figure 2a.
4. Calculate the density of the Na2He. Calculate the density of sodium at atmospheric pressure. How do they compare?
5. In the structure, each He and each interstitial 2e- is coordinated by eight Na atoms, so we can think about each of these as being in a cubic hole in a simple cubic unit cell. What is the radius ratio for a cubic hole (see a table of atomic radii)? Would each of these fit into the cubic hole?

**D. Electronic structure and other topics**

1. What is the source of the interstitial electrons?
2. How does band gap correlate to insulating properties? What experimental results were observed related to this? (See Figure 4a)
3. In Figure 3a, the solid blocks in the key correspond to the bottom of the figure, which are the predicted diffraction angles for the given elements. The three lines at the top are the actual spectra at the given conditions. In evaluating this figure, you should look at how the spectra change over the heating cycles. What peaks appear and disappear as the compound is heated at high pressure? How does this confirm the formation of the Na2He compound?
4. Figure 1a is similar to a Job’s Method plot. What would this graph look like if the stable compound had 2 He for every 1 Na instead of the stoichiometry that is observed?

1. Explain how the Na2He compound satisfies Pauling’s rules for ionic compounds.