Bonding in solids

1. **Bohr model.** Calculate the energy levels and radii of the corresponding orbits for the $n = 2$ and $n = 3$ states of hydrogen according to the Bohr model.

   The negative sign (-) is important. Why?

2. **Bohr model.** Derive the result of the Bohr model,

$$E_n = -\frac{m_e e^4}{8\epsilon_0^2 h^2 n^2}$$

   (a) Starting with the Coulomb force leads to the centripetal acceleration for circular motion

$$k\frac{|q|^2}{r^2} = m\frac{v^2}{r}$$

   determine the speed of the electron, $v = \ldots$

   (b) Determine an expression for the classical total energy of a proton-electron system. Start with

$$E = K + U = \frac{1}{2}mv^2 + k\frac{q^2}{r}$$

   substitute in $q_1 = +e$, $q_2 = -e$, and in your result from (a) to find E only in terms of r and some constants.

   (c) Add Bohr's main postulate that the electron's angular momentum $L = mvr$ is quantized as multiples of $\hbar$. That is,

$$L = mvr = n\hbar$$

   Substitute in your result from (a), then solve for r.

   (d) Combine (b) and (c) to find E_n.

   answers to arrive at: $v^2 = ke^2/mr$, $-e^2/8\pi\epsilon_0 r$, $r = (4\pi\epsilon_0)\hbar^2 n^2/me^2$

3. **electron configuration.** State the Pauli exclusion principle in your own words.

4. **electron configuration.** Calculate the number of electrons required to fill all of the energy levels up to and including the 4p subshell.

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5. **electron configuration.** Write down the ground state electron configuration of Na ($Z = 11$).

   The ground state electron configuration of N, for example, is $1s^2 2s^2 2p^3$.

6. **electron configuration.** Consider the following schematic of energy levels and filling in the different shells (from Harris)

   Use this chart to determine if the ionization energy will increase or decrease as the atomic number increases.

   For example:

   H → He: increase in ionization energy
   He → Li: large decrease in ionization energy
   Li → Be:

7. **electron configuration.** A simple extension of the Bohr model for other elements gives an energy of

$$E_n = -13.6\frac{Z^2}{n^2}\text{eV}$$

   (a) Calculate the ionization energy of He and Li.

   The gives a wrong value. The ionization energy of the $2s^1$ electron in Li (25eV) is actually lower than that of the $1s^2$ electron in He (5eV); starkly different from what's predicted. This is primarily due to *screening*, also referred to as *shielding*.

   (b) What is screening?

   (c) Why is screening more effective in Li than in He?

8. **electron configuration.** What are *valence electrons*? What are *core electrons*? Give a definition and one detailed example.

   Which electrons take part in the bonding process?

9. **electron configuration.** Consider the periodic table.

   (a) Identify the noble gases. These elements aren't very reactive. Do these elements have relatively large or relatively small ionization energies? Are these shells barely filled, almost filled, or fully filled?

   (b) Identify the Group IA elements (alkali metals). These elements are very reactive. Do these elements have relatively large or relatively small ionization energies? Are these shells barely filled, almost filled, or fully filled?

   (c) Identify the Group VII elements (halogens). These elements are very reactive. Do these elements have relatively large or relatively small ionization energies? Are these shells barely filled, almost filled, or fully filled?

10. **ionic bonding.** The potential energy of a single Cl^-ion in a NaCl crystal is 8.95eV. To find the lattice energy, we have to determine the potential energy for all the ions in the crystal. Let's say we have one mole of each ion.

    (a) Calculate the potential energy for one mole Cl^- ions.
    (b) Calculate the potential energy of one mole of Na^+ ions
    (c) It turns out that we've double counted when we did (a) and (b). So divide by each by 2, then add them. This will give the lattice energy in terms of eV/mol.
    (d) Change your result to kJ/mol.

    The lattice energy is the energy required to separate the crystal into separate ions.

    (860 kJ/mol)

11. **attractive and repulsive forces**. The interatomic forces can be modeled as

$$F = F_{\text{Coulomb}} + F_{\text{repulsion}} = -\frac{Aa_0^2}{r^2} + \frac{Ba_0^{10}}{r^{10}}$$

where a_0 is the *equilibrium* separation distance between atoms.

(a) Determine an expression for $U(r)$. Use the fact that $U(r) = -\int_\infty^r F(r)dr$.
(b) How are A and B related? Use the fact that a_0 is an equilibrium point.
(c) Graph $U(r)$. Identify a_0.

(Turton. You'll find that $A = B$.)

12. **attractive and repulsive forces.**

(a) The repulsive force is considered to be a short range force. Calculate the fractional change in the magnitude of $F_{\text{repulsion}}$ as the separation goes from a_0 to $2a_0$. Compare this the fractional change in the Coulomb force for the same separation, a_0 to $2a_0$.

(b) Calculate the percentage reduction in the lattice energy due to the inclusion of the repulsion term. Use your result from problem 10.

(Turton)

13. For each of the following, identify if it's likely have ionic bonding or covalent bonding:

H_2 hydrogen
LiF lithium flouride
KF potassium flouride
N_2 nitrogen
CH_4 methane
CO_2 carbon dioxide
H_2O water
NaCl sodium cloride
Na_2S sodium sulfide

Of course, you can look it up. Then, identify some criteria that will help you figure it out *without* having to ask someone else. Asking Google is asking someone else.

14. Describe, briefly, the mechanism behind metallic bonding.