

# Worked assignment 1: Bonding, DOS, and Fermi statistics

1. For a linear array of six hydrogen atoms, draw the six possible molecular orbitals in order of increasing energy. How does the energy depend on the number of nodes? Plot qualitative energy vs. bond length curves for this system and fill the level with appropriate number of electrons. What would you expect to be the equilibrium configuration of six H atoms?
2. Draw the energy vs. bond length curves for
  - (a) Ar
  - (b) NaCl
  - (c) Na
  - (d) Mg

Your diagram should highlight the fact that while Na and Mg are metals, Ar and NaCl are insulators.

3. There are 10 electrons in a slab that measures  $0.5(a) \text{ nm} \times 1(b) \text{ nm} \times 2(c) \text{ nm}$ . Each electron in the slab can be represented by a set of 3 quantum numbers  $(n_1, n_2, n_3)$ , which are positive integers (greater than zero) and are related to the energy of the slab and slab dimensions by

$$E = \frac{h^2}{8m_e} \left[ \frac{n_1^2}{a^2} + \frac{n_2^2}{b^2} + \frac{n_3^2}{c^2} \right]$$

- (a) Assign quantum numbers to the electrons
- (b) Deduce  $E_F$  from the energy distribution of electrons
- (c) Determine the density of states at  $E_F$ , including spin
- (d) What is the total kinetic energy of electrons in the slab?
- (e) What is the average kinetic energy of electrons in the slab?

4. Derive the expression for the density of states for a two dimensional solid and one dimensional solid. Compare this with the expression for a three dimensional solid.
5. Plot the Fermi function for temperatures of 0, 500, and 2000 K semi quantitatively and on the same plot. How accurate is the Boltzmann function as an approximation of the Fermi function when  $E - E_F = 3k_B T$  and  $E - E_F = 15k_B T$ ?