Structure of Matter - II
June 17, 2014

PROBLEM 1. Molecules [20 pts]

Give a concise, precise description of

a) the Born-Oppenheimer approximation, [1 pts]
b) hybridization, [1 pts]
c) Frank-Condon transitions, [1 pts]
d) why an electronic transition between two electronic states which are both in their vibrational ground state is unlikely, [1 pts]
e) and why a 2-state system cannot be a laser. [2 pts]

Consider the O-based triatomic atoms OX_2 and OY_2. In OX_2 the bonds are based on sp^3 hybrid orbitals while in OY_2 the bonds are based on sp hybrid orbitals.

f) Which one of the molecules is linear and why? [3 pts]
g) Somewhere within the whole series of the rotational energy levels of the linear molecule, there are 3 consecutive rotational levels that have energies of 112, 144, and 180 cm^{-1}. Determine the rotational constant $\tilde{B}$ (in units of cm^{-1}) and the J values of these levels. Note that when using cm^{-1} as energy unit hc=1. [2 pts]
h) How does the rotational spectrum change if either the O or one of the other two atoms is replaced by a heavier isotope of the same species. You may assume that internuclear distances do not change. [3 pts]

Consider a heteronuclear diatomic molecule AB. The bonding orbital of the molecule is given by $\psi = 6\phi_A + 8\phi_B$

i) Normalize the wavefunction. [1 pts]
j) Determine the charge imbalance between A and B. [2 pts]
k) Is the molecule polar and does it have an electric dipole moment [1pts]
l) What is the wavefunction of the antibonding orbital. [2 pts]

PROBLEM 2. Solid state [20 pts]

Give a concise, precise description of

a) the Born-von Karman boundary condition, [1 pts]

b) phonons, [1 pts]

c) an intrinsic semiconductor, [1 pts]

d) the functioning of an acceptor doped semiconductor crystal, [2 pts]

e) and, a p-n junction. [2 pts]

Consider a simple 2D square lattice with the atomic lattice distance equal to b. The sides of the full crystal are of length L. L is much, much larger than b.

f) Calculate the areas of the Wigner Seitz cell and first Brillouin zone cell. [2 pts]

Now consider the crystal to be a free-electron metal. To describe the electron gas we assume it to be confined in a 2D square well with infinite walls at x=0 and L and y =0 and L.

g) Show that ψ = A $\sin(\frac{n_x \pi}{L} x) \sin(\frac{n_y \pi}{L} y)$ is a solution. [1 pts]

h) Find the expression for the energy E_n of the free-electron gas with n defined as $n = \sqrt{n_x^2 + n_y^2}$. [1 pts]

i) In this square well we accommodate N electrons. Determine the expression for the Fermi energy. [2 pts]

j) Calculate the Fermi energy in eV for N=10^{12} electrons per cm^2. [1 pts]
Hint: $\hbar$ = 1.05 x 10^{-34} Js, m_e= 9.11 x 10^{-31} kg

k) Determine the density of states D(E). [2 pts]

l) What happens to the Fermi energy when the atomic lattice distance in one of the directions is changed from say b to b/2. [2 pts]

m) In reality the 2D crystal is not infinitesimal thin but has a certain thickness d. Estimate the maximal thickness d for which the crystal may still be considered to be a 2D free-electron metal. [2 pts]