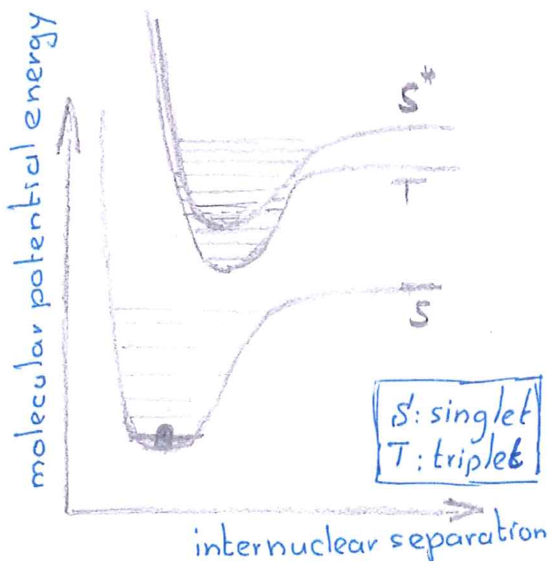
Structure of Matter - II
July 7, 2014

PROBLEM 1. Molecules [20 pts]



Give a concise, precise description of

a) the Born-Oppenheimer approximation, [1 pts]
b) a Π_g orbital (add sketch and mention whether the orbital is bonding or antibonding), [1 pts]
c) and, on basis of the figure, the (sequence of) processes leading to phosphorescence after photon absorption. Redraw the figure and include (schematically) all the processes from absorption to phosphorescence. Initially the molecule is in its ground vibrational state. [3 pts]

Consider a triatomic molecule, XY_2.

d) The bonds are based on sp hybridized orbitals. What is the geometrical shape of the molecule? [2 pts]
e) Somewhere within the whole series of the rotational energy levels of the molecule, there are 3 consecutive rotational levels that have energies of 56, 72, and 90 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]
f) Now the atom X is replaced by one of its heavier isotopes. Can the rotational spectrum be used to determine the location of X in the molecule and why? [2 pts]
g) The molecule is infrared active. What is the relevant selection rule. [1 pts]
   Hint: Between which kind of states do infrared transitions occur.
h) From the infrared activity can one determine the location of X in the molecule? [2pts]

Consider a heteronuclear diatomic molecule AB. The bonding orbital of the molecule is given by $\psi = 2\phi_A + 3\phi_B$. The wavefunctions ϕ_A and ϕ_B are real.

i) Normalize the wavefunction for the case that the overlap integral is 0.25. [2 pts]
j) Determine the charge imbalance between A and B. [2 pts]
k) For the case of the overlap integral being 0, determine the wavefunction of the antibonding orbital. [2 pts]

PROBLEM 2. Solid state [20 pts]

Give a concise, precise description of

a) phonons, [1 pts]

b) an intrinsic semiconductor, [2 pts]

c) the functioning of a donor doped semiconductor crystal, [2 pts]

d) and, the occurrence of a depletion zone in a p-n junction. [2 pts]

Consider a simple 3D square lattice with the atomic lattice distance equal to a.

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

f) Consider the planes described by the Miller indices (2,1,1). Determine the distance between these planes. [2 pts]

Consider a 2D free-electron metal with a simple square lattice with the atomic lattice distances equal to a. The sides of the full crystal are of length L. L is much, much larger than a. To describe the electron gas we use traveling waves in such a way that the wavefunction is given by: $\psi = Ae^{ik_x x}e^{ik_y y}$ with $k_i = \frac{2\pi}{L}n_i$ and i=x,y.

g) Show that ψ meets the periodicity (or Born-von Karman) condition. [1 pts]

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

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

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

k) What happens to the Fermi energy when the atomic lattice distance in one of the directions is changed from say a to a/2. The size of the crystal is kept constant.[2 pts]