PROBLEM 4. [5 pts]

Consider a triatomic molecule, XY_2. Its bonds are based on sp hybridized orbitals.

a) What is the geometrical shape of the molecule? [1 pts]

b) 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]

c) Now the atom X is replaced by one of its heavier isotopes. Can the rotational spectrum be used to find out the location of X within the molecule and how? [2 pts]

PROBLEM 5. [6 pts]

Give a concise, precise description of

a) an intrinsic semiconductor at T=0 and at T>0, [2 pts]

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

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

PROBLEM 6. [4 pts]

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

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

b) Consider the planes described by the Miller indices (2,3,1). Determine the distance between these planes. [2 pts]

PROBLEM 7. [8 pts]

Consider a 2D free-electron metal with a simple rectangular lattice with the atomic lattice distances being a and 2a, respectively. The full crystal as a whole is square-shaped with sides of length L. L is equal to 10^5 a. To describe the electron gas traveling waves are used. Their wave function 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.

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

b) Use to the Schrödinger equation to 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]

c) Each atom in the crystal donates one electron to the free-electron gas. Determine the Fermi energy in units of $\frac{\hbar^2}{ma^2}$. [2 pts]

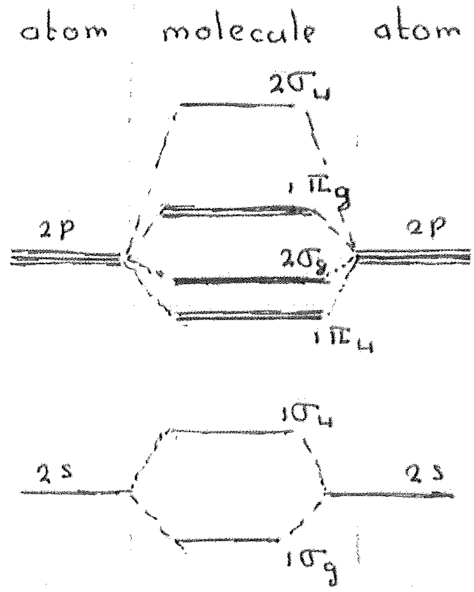
d) How does to Fermi energy compare to the lowest reciprocal lattice energy [2 pts]

e) 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]

Freddie Hendriks

Structure of Matter – 2 **June 18, 2015**

PROBLEM 1. [7 pts]



Consider the B_2 molecule. The electronic configuration of a single B atom is $1s^2 2s^2 2p$. The figure shows the relevant molecular orbital energy level diagram.

a) Redraw the figure and indicate the electronic population of the molecular orbitals, use ↑ and ↓ for spin up and down, respectively. [2 pts]

b) Which one of the following molecules B_2^-, B_2, and B_2^+ has the highest dissociation energy, and why? [1 pts]

c) Give the electronic configuration of the B_2 molecule, [1 pts]

d) Determine the term symbol of the ground electronic configuration, [3 pts]

PROBLEM 2. [5 pts]

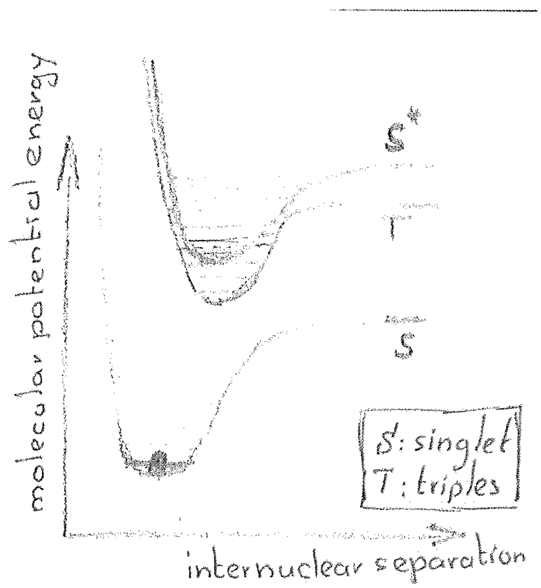
Consider a heteronuclear diatomic molecule AB. The bonding orbital of the molecule is given by $\psi = 3\phi_A + 2\phi_B$. The wavefunctions ϕ_A and ϕ_B are real.

a) Normalize the wavefunction for the case that the overlap integral is 0.25. [2 pts]

b) Determine the charge imbalance between A and B. [1 pts]

c) For the case of the overlap integral being 0, determine the wavefunction of the antibonding orbital. [2 pts]

PROBLEM 3. [5 pts]



Consider now a solvated molecule in its ground vibrational state. The lowest molecular orbitals are sketched in the figure.

a) Give a description of the (sequence of) processes leading to phosphorescence after photon absorption. Redraw the figure and include (schematically) all the processes from absorption to phosphorescence. [3 pts]

b) The molecules are to be used as a laser medium, indicate which transition you would use as laser transition, and why. [2 pts]