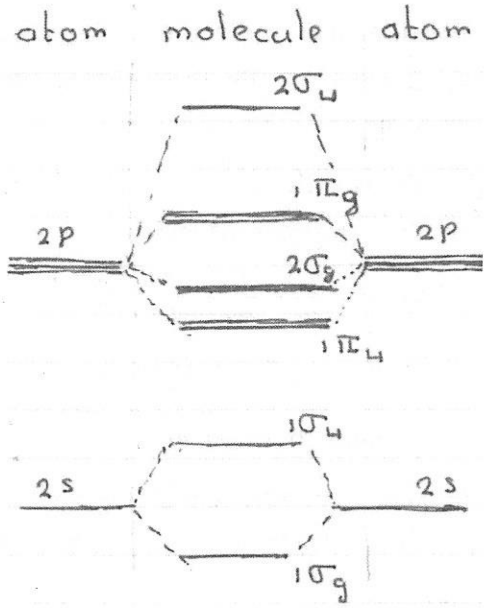
Structure of Matter – 2 **June 16, 2016**

PROBLEM 1. [6 pts]



Consider ~~the two-fold charged~~ B_2 molecule. The electronic configuration of a B atom is $1s^2 2s^2 2p$. The figure shows the relevant generic 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. [1 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]

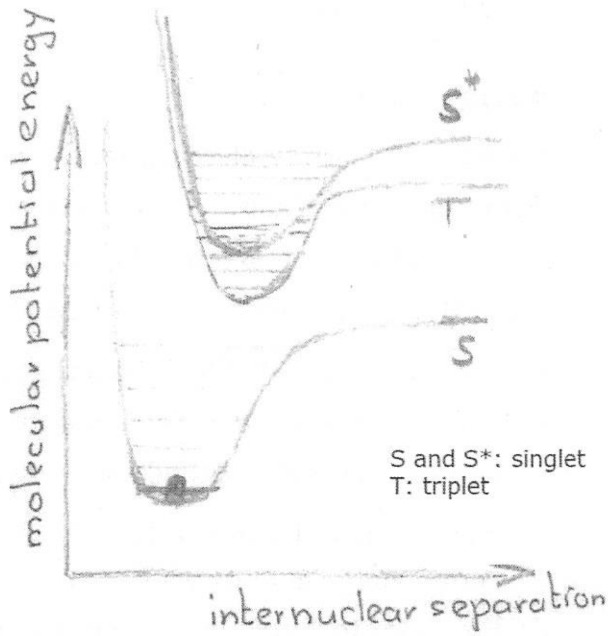
PROBLEM 2. [4 pts]

Consider a heteronuclear diatomic molecule AB. The bonding orbital of the molecule is given by the normalized wavefunction $\psi = \frac{2\phi_A + 3\phi_B}{4}$. The wavefunctions ϕ_A and ϕ_B are real.

a) Determine the value of the overlap integral. [2 pts]

b) Determine the charge imbalance between A and B. [2 pts]

PROBLEM 3. [7 pts]



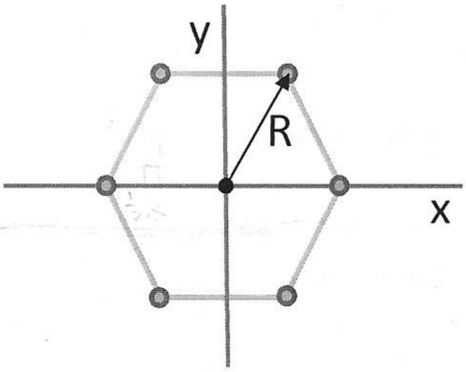
Consider now a solvated molecule in its ground vibrational state. The lowest molecular orbitals are sketched in the figure.

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) How do the processes change if the molecules are taken out of the solution and brought into vacuum and why. [2 pts]

c) We want to use these molecules for making a laser. Should the molecules be placed in vacuum or rather in solution, and why [2 pts].

PROBLEM 4. [7 pts]



Consider a C_6 molecule as depicted.

a) Determine the moment of inertia about the figure axis ($\equiv I_{\parallel}$) [1 pts]

b) Show that $I_x = I_y$ ($\equiv I_{\perp}$) [2 pts]

c) The energies of the pure rotational levels are given by $E = \frac{J_x^2}{2I_x} + \frac{J_y^2}{2I_y} + \frac{J_z^2}{2I_z}$ with J_i the angular momenta.

Show that for C_6 the energies can be expressed by $E = \frac{J^2}{2I_{\perp}} + (\frac{1}{2I_{\parallel}} - \frac{1}{2I_{\perp}})J_z^2$ with J the total angular momentum. [1 pts]

d) In the following assume atomic units, thus : M_{Carbon} = 12; R=2; and ħ=1. Determine the energies of the 3 lowest rotational levels [3 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 an acceptor doped semiconductor crystal, [2 pts]

c) and, the occurrence of a band gap in an intrinsic semiconductor. [2 pts]

PROBLEM 6. [4 pts]

Consider a rectangular 3D lattice with the atomic lattice distances in x, y, and z direction equal to a, 2a and 3a, respectively.

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

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

PROBLEM 7. [6 pts]

Consider a 2D free-electron metal with a rectangular lattice with the atomic lattice distances being a and 0.5a, respectively. The crystal as a whole is square-shaped with sides of length L. L is equal to 10^5 a. To describe the electron gas standing waves are used. Their wave function is given by: $\psi = A\sin(k_x x)\sin(k_y y)$ with $k_i = \frac{\pi}{L} n_i$ 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 energy state of the reciprocal lattice. [2 pts]