Please limit your answer to maximum 5 min (+ 5 min for questions)

Exercise 2.1 (Molecular Orbitals)

Please describe (preferably as a PPT presentation with 3-4 slides):

- The orbitals of a cyclic aromatic compound with N atoms are described by the Coulson formula:

$$E_q = \alpha + 2\beta \cos\left(\frac{2\pi q}{N}\right) \qquad q = 1,2,\ldots N$$

$$\psi_q = \sum_{n=1}^{N} a_n^q \psi_{2p_z}(n) \qquad a_n^q = \sqrt{\frac{1}{N}}\, e^{\left(\frac{2i\pi qn}{N}\right)}$$

a) Calculate the energies of the π molecular orbitals of benzene and represent them in an energy level diagram.

b) Applying the Pauli exclusion principle, calculate the energy lowering of the system (as compared to the isolated carbon atoms) induced by the bonding of the π electrons.

c) Calculate the wavefunctions with highest and lowest energy and sketch all the Hückel molecular orbitals.

Hint: the remaining wavefunctions are given by

$$\psi_5 = \frac{1}{\sqrt{12}}(2\psi_{p_z}(1) + \psi_{p_z}(2) - \psi_{p_z}(3) - 2\psi_{p_z}(4) - \psi_{p_z}(5) + \psi_{p_z}(6))$$

$$\psi_1 = \frac{1}{2}(\psi_{p_z}(2) + \psi_{p_z}(3) - \psi_{p_z}(5) - \psi_{p_z}(6))$$

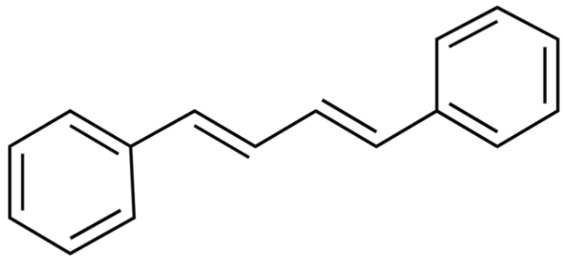
$$\psi_2 = \frac{1}{\sqrt{12}}(2\psi_{p_z}(1) - \psi_{p_z}(2) - \psi_{p_z}(3) + 2\psi_{p_z}(4) - \psi_{p_z}(5) - \psi_{p_z}(6))$$

$$\psi_4 = \frac{1}{2}(\psi_{p_z}(2) - \psi_{p_z}(3) + \psi_{p_z}(5) - \psi_{p_z}(6))$$

Exercise 2.2 (Particle in a box)

Please describe (preferably as a PPT presentation with 3-4 slides):

The molecule 1,4-Diphenyl-1,3-butadiene has an absorption maximum of 350 nm.



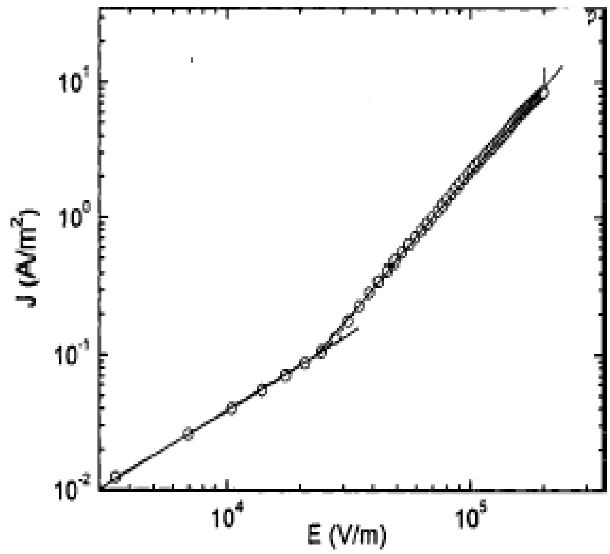
a) Calculate the lowest energy absorption wavelength of 1,4-Diphenyl-1,3-butadiene using the particle in a box model. You can assume that the phenyl rings are the confining walls representing the "box".
b) How does the calculated value compare to the experimental value?

($m_{electron}$=9.1·10^{-31} kg, c=3·10^{8}·ms^{-1}, h = 6.62·10^{-34} Js, C=C bond length 133 pm; C-C bond length 154 pm)

Exercise 2.3 (Mobility)

Please describe (preferably as a PPT presentation with 3-4 slides):

a) Estimate the charge carrier mobility in a conjugated organic single crystal from the current-voltage plot on the right. The data was obtained by sandwiching the 20 μm thick crystal between two gold electrodes. First determine which region of the current-voltage characteristics is governed by ohmic behavior and which is governed by space charge limited current. Explain why.



b) You expect to have measured the hole or electron mobility?

(Take ε=3 as the dielectric constant of the molecular solid)

c) How will the curve change in the presence of traps?

Exercise 2.4. (Solar Cell Efficiency)

Please describe (preferably as a PPT presentation with 3-4 slides):

A solar cell is fabricated with an organic semiconductor that absorbs from 350 nm to 600 nm. The semiconductor has a maximum extinction coefficient of 100’000 l $mol^{-1}cm^{-1}$. A thin solid film of the organic semiconductor is fabricated by evaporation in vacuum and has an absorbance of 0.5 at the maximum. The molar mass of the material is 1.5g/cm^3 and 300 g/mol, respectively.

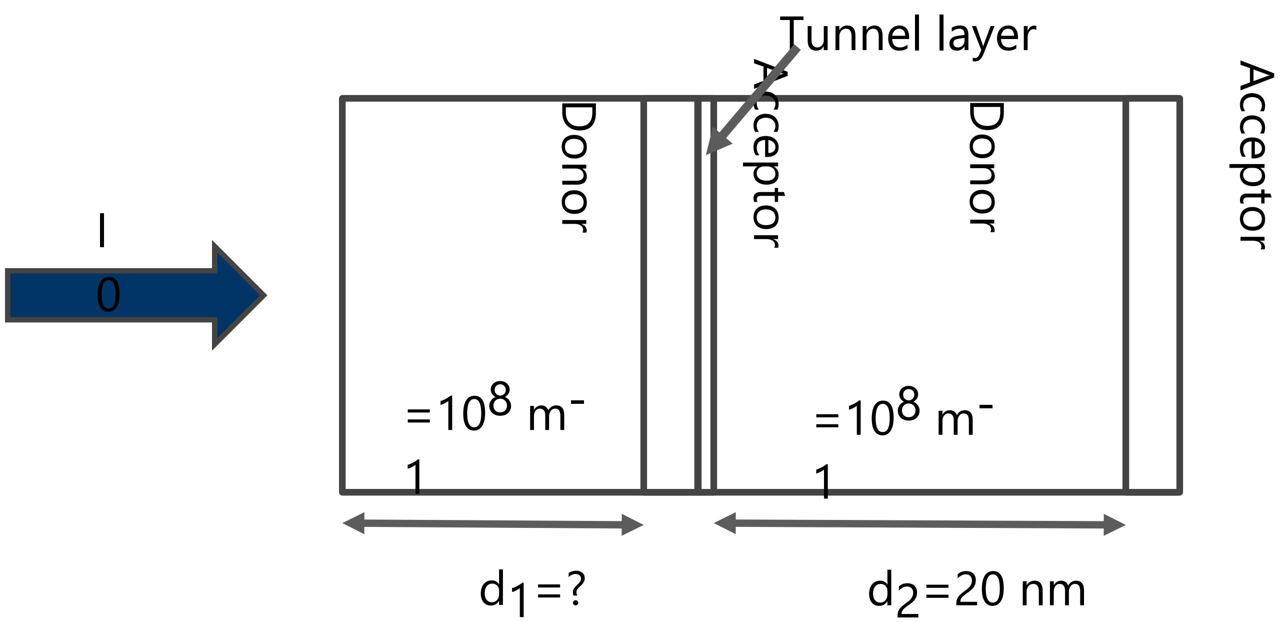
a) Estimate the thickness of the film.
b) What is the maximum short-circuit current density that could be delivered by this solar cell at AM 1.5 solar irradiation. Hint: roughly estimate the number of photons that are absorbed by the cell, take absorbance and absorption wavelength range into account.
c) What is the maximum cell efficiency, assume that the optical bandgap defines the maximum possible photovoltage, ($h = 6.63 \cdot 10^{-34}$ Js; $c = 3 \cdot 10^{8}$ m/s; use a fill factor of 0.7)

Exercise 2.5. (Tandem solar cell and current matching)

Please describe (preferably as a PPT presentation with 3-4 slides):

Due to the short exciton diffusion length, bi-layer organic solar cells cannot be very thick. One strategy to enhance absorbance is to stack two bilayer cells on top of each other.

a) The back cell has a thickness of d_2 = 20 nm, which corresponds to the exciton diffusion length. The absorption coefficient of the donor material is $\alpha = 10^8\ m^{-1}$. As the cells are connected in series, it is necessary to match the currents of the front and back cell. You may assume that the acceptor and tunnel layers do not absorb any light, the tunnel-junction is ideal and the charge collection efficiency is 100%. How thin does the front cell need to be?

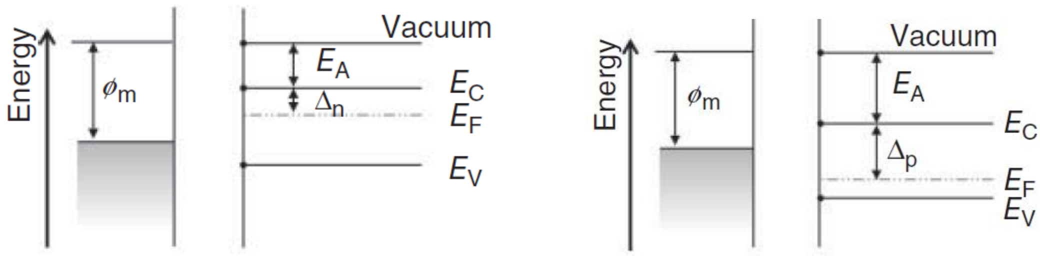


Exercise 2.6 (Metal Organic Contact)

Please describe (preferably as a PPT presentation with 3-4 slides):

In so-called Schottky Organic Solar Cells, a diode characteristic is realized by band-level alignment at the metal/organic interface.

a) Explain the phenomena of band bending and plot an energy diagram when a n-type and p-type organic semiconductor are brought into contact with the metal in the figure below.
b) Also draw charge distribution and electrical field strength across the interface.
c) Which parameters determine the width of the interface?



Energy levels of n-type and p-type semiconductors

Exercise 2.7 (Stability of Perovskite Solar Cells)

Please describe (preferably as a PPT presentation with 3-4 slides):

Degradation in Perovskite solar cells is still one of the main challenges to tackle.

a) Why in perovskite a "mixed" cation approach is frequently followed? (Lit: G. Han et al., J. Phys. Chem. C 2018, 122, 13884−13893).

   One issue concerns structural stability of the perovskite crystal. Explain the concept of "tolerance factor", calculate the tolerance factors for $MAPbI_3$, $NaPbI_3$, and $EDAPbB_3$ and explain with these examples how that is related to structural stability.

b) E. T. Hoke et al. (Chem. Sci., 2015, 6, 613–617) described a reversible photoinduced trapping effect.

   Please explain how this effect can be understood. Detail the various arguments that are used to underline the interpretation of the authors.