Please limit your answer to maximum 7 min (+ 3 min for questions)

Exercise 3.1 (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:



1. Calculate the energies of the  molecular orbitals of benzene and represent

 them in an energy level diagram.

1. 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  electrons.

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

Hint: the remaining wavefunctions are given by

$$\begin{array}{c}ψ\_{5}=\frac{1}{\sqrt{12}}(2ψ\_{p\_{z}}(1)+ψ\_{p\_{z}}(2)-ψ\_{p\_{z}}(3)-2ψ\_{p\_{z}}(4)-ψ\_{p\_{z}}(5)+ψ\_{p\_{z}}(6))\\ψ\_{1}=\frac{1}{2}(ψ\_{p\_{z}}(2)+ψ\_{p\_{z}}(3)-ψ\_{p\_{z}}(5)-ψ\_{p\_{z}}(6))\end{array}$$

$$\begin{array}{c}ψ\_{2}=\frac{1}{\sqrt{12}}(2ψ\_{p\_{z}}(1)-ψ\_{p\_{z}}(2)-ψ\_{p\_{z}}(3)+2ψ\_{p\_{z}}(4)-ψ\_{p\_{z}}(5)-ψ\_{p\_{z}}(6))\\ψ\_{4}=\frac{1}{2}(ψ\_{p\_{z}}(2)-ψ\_{p\_{z}}(3)+ψ\_{p\_{z}}(5)-ψ\_{p\_{z}}(6))\end{array}$$

Exercise 3.2 (Metal Organic Contact)

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

When an organic semi-conductor is contacted to a metal, either an Ohmic or a Schottky contact is formed.

1. Explain the phenomena of band bending and plot an energy diagram when a n-tpye and p-type organic semiconductor are brought into contact with a metal.
2. Also draw charge distribution and electrical field strength across the interface.
3. How does an I-V curve look compared to an Ohmic contact?
4. What does that mean for charge extraction?

Literature: Web sources like Wikipedia, script

N. Chander, S. Singh, S. S. Kumar Iyer, Stability and reliability of P3HT:PC61BM inverted organic solar cells, Solar Energy Materials & Solar Cells 2017, 161, 407–415. DOI: 10.1016/j.solmat.2016.12.020

Exercise 3.3 (Crystal growth in Perovskites)

Crystal growth of perovskite films can be tuned by control of either nucleation or growth.

1. Explain the classical theory of nucleation and growth with the help of a free energy diagram. Explain the terms critical free energy and critical radius of a nucleus for perovskites.
2. Describe two strategies that are followed today to control nucleation and crystal growth in perovskites.

Literature:

Lee J-W, Lee D-K, Jeong D-N, Par N-G, Control of Crystal Growth toward Scalable Fabrication of Perovskite Solar Cells, Advanced Functional Materials 2018, 29 (47), 1807047, DOI: 10.1002/adfm.201807047

Kumar J, Srivastava P and Bag M, Advanced Strategies to Tailor the Nucleation and Crystal Growth in Hybrid Halide Perovskite Thin Films. Front. Chem. 2022,10, 842924. DOI: 10.3389/fchem.2022.842924

Exercise 3.4 (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.

1. How do defects in perovskite solar cells impact performance and stability?
2. Describe a couple of strategies that are followed to passivate defects.
3. One issue concerns structural stability of the perovskite crystal. Explain the concept of "tolerance factor", calculate the tolerance factors for MAPbI3, NaPb I3, and EDAPbB3 and explain with these examples how that is related to structural stability.

Literature:

Wang, Z.; Gao, H.; Wu, D.; Meng, J.; Deng, J.; Cui, M. Defects and Defect Passivation in Perovskite Solar Cells. Molecules 2024, 29, 2104. DOI: 10.3390/molecules29092104

G. Han et al., Additive Selection Strategy for High Performance Perovskite Photovoltaics, J. Phys. Chem. C 2018, 122, 13884−13893: DOI: 10.1021/acs.jpcc.8b00980