

**Organic Electronic Materials 2025 Exercise 2 (submit on 21.03.25)**

1. **Homework** – In the paper “Week 2 Slater 1965 Molecular Orbitals”, Slater compares both the valence bond and molecular orbital theory. What is the difference between both models in terms of interactions involved in them? Illustrate this difference with the example of a diatomic molecule that has 2 electrons in total.
2. Draw a schematic MO energy level diagram as well as pictorial representations of the resulting MO for the interaction of two helium atoms. Name the AO and MO and add the electrons. Explain the terms “bonding” and “antibonding” MO. Explain why  $\text{He}_2$  is not stable, and give a quantitative expression for the destabilization energy of  $\text{He}_2$  compared to two He atoms.
3. Draw the MO energy level diagram of the C=C double bond in ethene. Start by briefly explaining which atomic orbitals or hybridized orbitals are involved in the double bond and why the chosen hybridization is required. Briefly explain the difference between  $\sigma$ -bonds and  $\pi$ -bonds, and draw graphical representation of the molecular orbitals.
4. Give the Hückel matrices for 1,3-butadiene and 1,3-cyclobutadiene (a linear and a cyclic  $\pi$ -system with four carbon atoms). Why are they different? Draw the MO energy level diagram of both systems and explain the difference in stability. What is aromaticity?
5. Give the formula for the energy values of linear  $\pi$ -conjugated systems according to the Hückel theory. Draw the MO energy diagram of the  $\pi$ -system of 1,3,5, 7-octatetraene as an example. Give the energy values of the different MO levels. Include simplified graphical representations of all MO (hint: consider the node planes).
6. Draw schematic MO energy level diagrams for the  $\pi$ -systems of ethene, 1,3-butadiene, 1,3,5-hexatriene, and the limiting case of polyacetylene. Include only the  $\pi$  molecular orbitals (not the constituting AOs). Explain why polyacetylene doesn't strictly follow Hückel theory.

**Further Reading:**

Clayden, Greeves & Warren, *Organic Chemistry*, **2012**; “Chapter 7 – Delocalization and Conjugation”.

Nordholm et al., “The Mechanism of Covalent Bonding”, *J. Chem. Ed.* **2007**, 84, 1201.

Fox et al., “Electronic Structure in  $\pi$ -Systems”, *J. Chem. Ed.* **1985**, 62, 367 (just the first two pages).