School of Engineering
Institute of Materials
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and Organic Materials

Organic Electronic Materials 2025 Exercise 5 (submit on 04.05.25)

1. Using qualitative energy diagrams, represent the energy landscapes of polyacetylene and polythiophene, and draw the molecular structures corresponding to their different states. What is the difference between the ground states of these two polymers?
2. Draw the MO energy level diagrams of both polymers of question 1 when doped with a very small amount of an oxidant, and name the species formed in both cases. Draw their chemical structures and define what they are from an organic chemistry perspective.
3. Describe qualitatively with your own words Peierls' distortion and what this causes in polyacetylene.
4. What are the characteristics of a soliton? What experimental technique provides strong evidence for its presence, and how does it work?
5. What different factors may influence the correlation length of polarons/bipolarons?
6. Molecular flexibility affects the dynamic disorder in organic semiconductors which can in turn limit the delocalization of charge carriers. With the help of energy band diagrams and example molecular structures, explain why this happens.
7. Draw the energy band diagrams of (i) a highly doped crystalline organic semiconductor and (ii) a highly doped amorphous organic semiconductor. Explain why you would expect the overall conductivity of the amorphous system to be lower than the crystalline system (assuming the same molecule and same operating temperature in both systems).

Reading suggestions:

- Electronic Processes in Organic Semiconductors: An Introduction (A. Köhler and H. Bässler, Wiley VCH 2015), Chapter 3.3: **Charge Carrier Transport**.
- Organic Electronics II (H. Klauk, Wiley VCH 2012), Chapter 3: **Charge Transport Theories in Organic Semiconductors** (R. Noriega, A. Saleo).
- V. Coropceanu *et al.*, *Chem. Rev.* **107**, 926, (2007); **Charge Transport in Organic Semiconductors**.

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