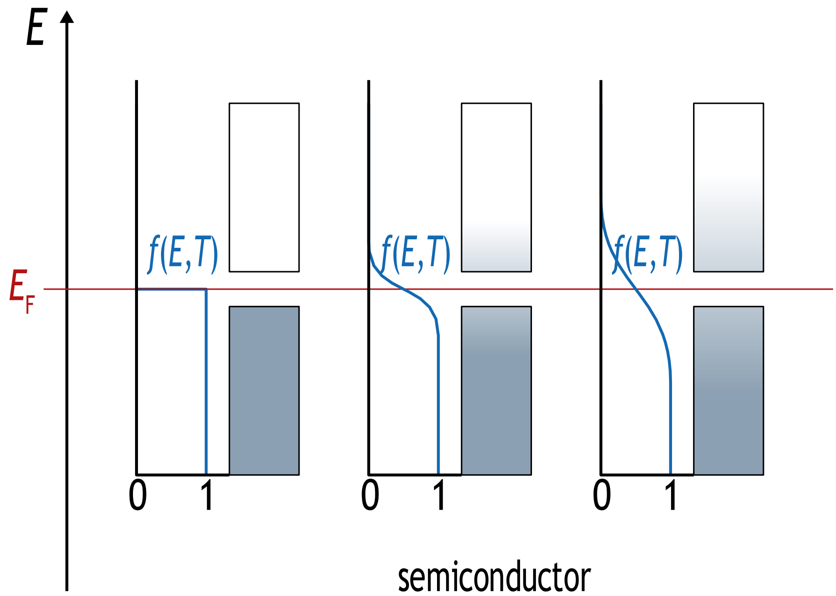
School of Engineering
Institute of Materials
Laboratory of Macromolecular
and Organic Materials

Organic Electronic Materials 2025 Exercise 6 (submit on 25.05.25)

Solutions

1. Sketch graphs showing the density of occupied states with energy for a material at (i) 0 K, and (ii) at 300 K. Label the Fermi energy level in each graph. Why is the density of mobile charge carriers for intrinsic transport in a pure organic semiconductor *much* lower than for pure silicon?



The density of mobile charge carriers in a pure organic semiconductor is much lower than for pure silicon because the band gap is larger, so at the similar temperatures, the first levels of the conduction bands in organic semiconductors have a lower occupation probability than in pure silicon.

2. Considering the data on the slide titled "Typical Electrode Materials and Organic Semiconductors" in 5.4:
   a. Which electrode material would you choose between gold and aluminum to get an injection into a layer of cyano-perylene derivative without resistance?
   Aluminum should be chosen as it would theoretically allow for injection of electrons without resistance.
   b. Which carrier type is aluminum more prone to inject into a layer of rubrene (5,6,11,12-

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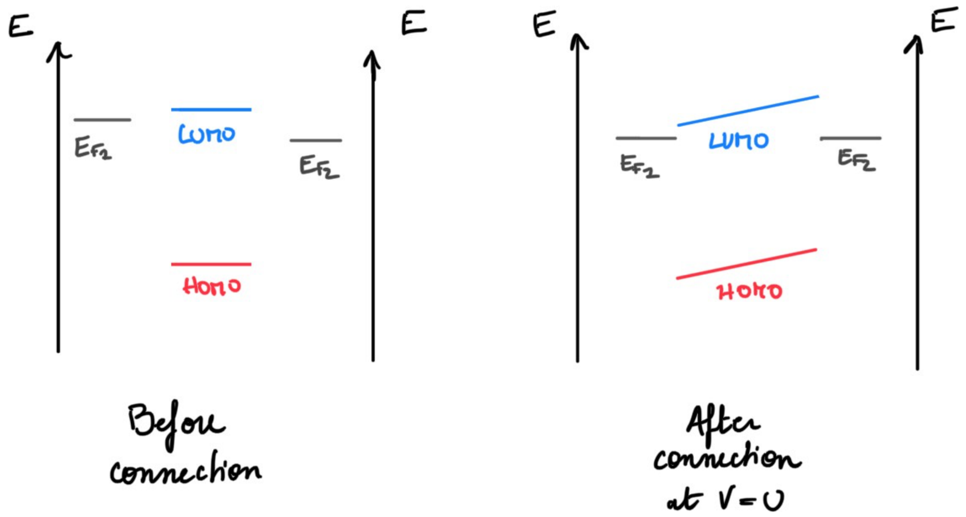
tetraphenyltetracene)?

Aluminum cannot inject electrons or hole in rubrene without resistance. However, as the work function of aluminum is closer to the LUMO than the HOMO in energy, the energy cost is lower for injection of electrons, which it is therefore more prone to inject.

3.

a. Draw the energy diagram of a simple one-layer electron transport-only device, i.e. a layer of organic semiconductor sandwiched between two suitable electrodes. *Note: We consider that we cannot find electrodes that would lead to injection of electrons into the organic semiconductor without resistance.*

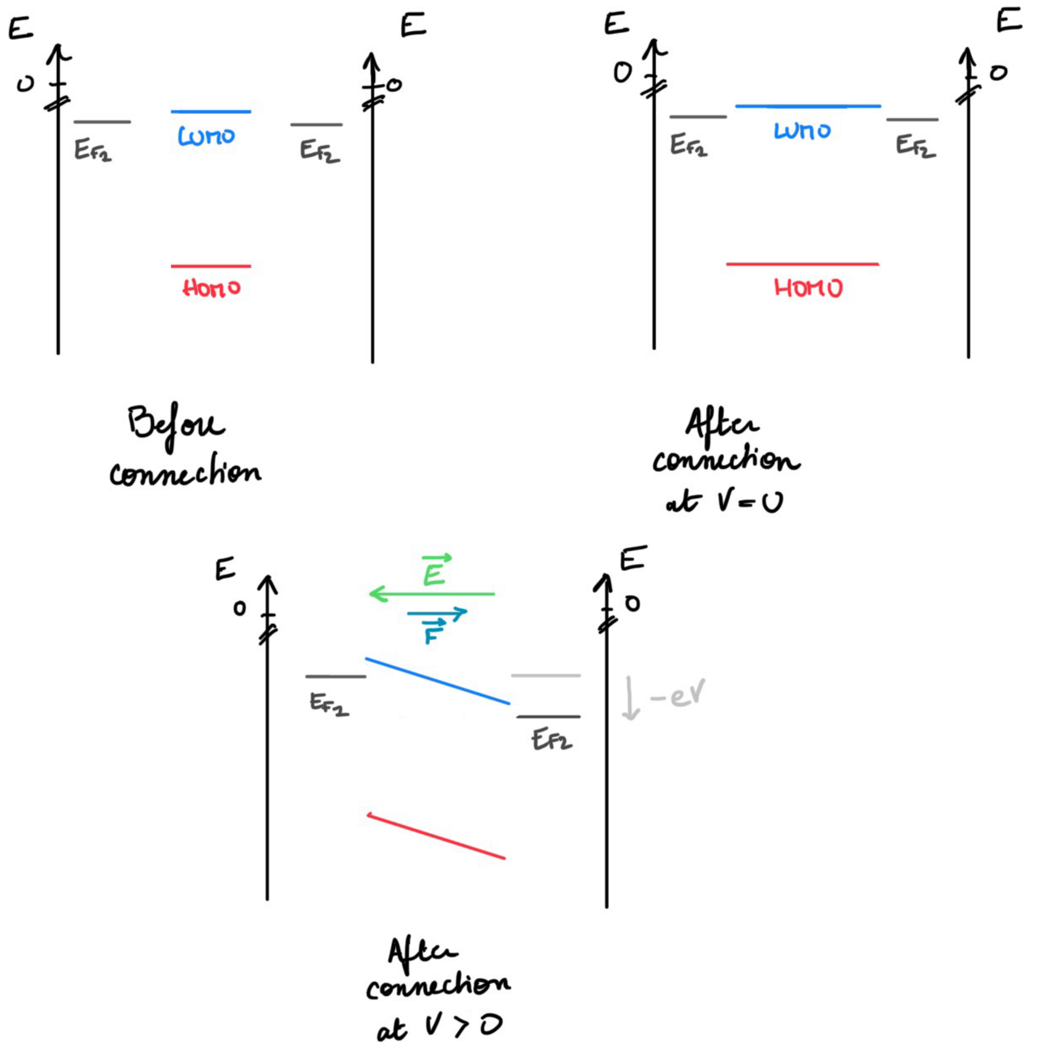


By choosing electrodes with fermi levels around the LUMO level of the organic semiconductor sandwiched in between, only electrons flow on the LUMO will participates to the current in the device.

b. Give the diffusion (or built-in) potential in the case where both electrodes are the same.

When both electrodes are identical, $V_{bi}=0$

c. In the former case of identical electrodes, draw the energy diagram of the device after application of a positive potential on the Fermi level of the right electrode. *Note: The Fermi level of the left electrode is fixed.*



Applying a positive voltage of the right electrode effectively shift it's Fermi level of qV with q=-e (since electrons are constituting the electrode), so it lowers it. This electrode becomes then effectively less charged (there is less electrons or they are deeper in energy, so require more energy to move) than the left one.

d. Considering the relation between gradient of potential and electric field, draw the electric field thus created, directly on your previous drawing.

An electric field is oriented from the less charged region to the more charged one: $\vec{E} = -\overrightarrow{grad}(V)$. *Therefore, in our case,* $\vec{E}$ *is oriented from the right electrode to the left one.*

e. Give the expression of the force created by an electric field on an electron.

$$\vec{F} = q\vec{E} \text{ with } q = -e$$

f. From which electrode, left or right, would the electrons be injected into the organic semiconductor layer? Explain why.

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The electric field created by the application of a positive voltage on the right electrode induce a force on the electrons that urges them to move from the left electrode to the right, so electrons are injected into the organic semiconductor layer from the left electrode.

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