School of Engineering
Institute of Materials
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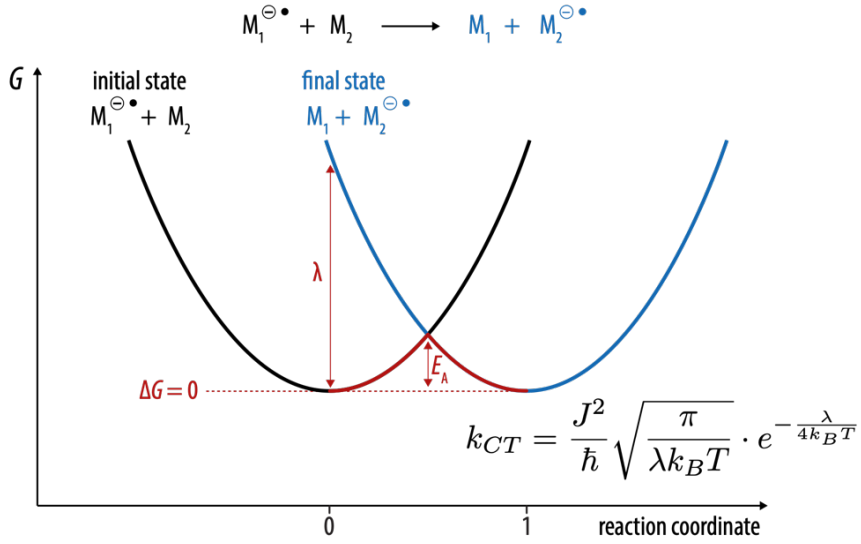
Organic Electronic Materials 2025 Exercise 7 (submit on 25.05.25)

Solutions

1. Which term of the one-electron Hamiltonian for charge transport has to dominate for band transport in organic materials? Justify this answer by explaining what is happening when this term dominates to both the energy levels of each energy site of the system and the electrons.

Both the excitation and electron transfer term of the one-electron Hamiltonian have to dominate for band transport in organic semiconductors. Indeed, in this case most molecules are coupled, the energy levels of all the molecules (or separated energy sites) involved are recombined, leading to a smaller band gap but most of all, bands of available energy on each molecule instead of singular energy level and a delocalization of the electrons over the molecules involved, which ease their transport.

2. 'Hopping' is one of the main incoherent charge transport mechanisms in organic semiconductors. Justify this terminology by briefly explaining how it works with the help of an energy state diagram. Include in your explanation how the temperature is related to the mechanism.



This terminology of "hopping" is justified because it refers to a transport mechanism in which a charge carrier (put in movement by a force that we don't need to discuss here)

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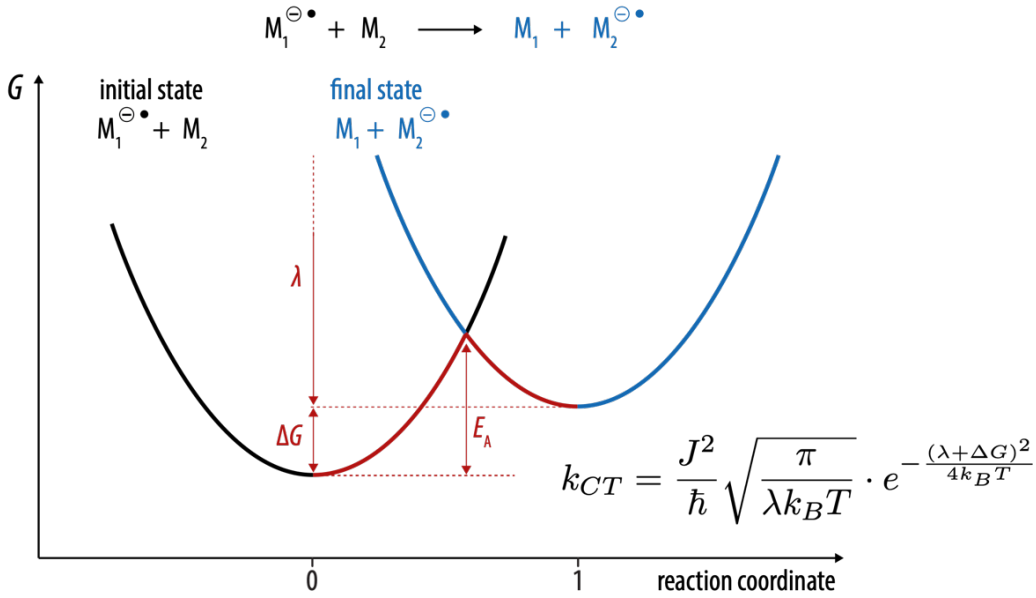
reaches a neighboring energy site by overcoming an energy barrier. Therefore, this process requires to be assisted by external energy, like thermal energy and, an increase in temperature leads to an enhance mechanism.

3. Why do the transfer steps in disorder-controlled charge transport become asymmetric?

In disorder-controlled charge transport, the energy levels can be different on each site leading to transfer steps that might be easier in one direction than the other.



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4. How does charge transport occur in the "multiple trap and release" (MTR) model? Describe the two competing (in fact, opposing) effects of the temperature on mobility according to this model.

In the "multiple trap and release" model, charge transport alternates between hopping between localized states, also named "traps", and band like transport over delocalized states after random hopping on one on these delocalized states and before being trapped again by a localized state. Increasing the temperature has two opposite effects on the mobility in this model, since it increases the transport rate in hopping but reduces it in band like transport, and reversibly for decreasing the temperature.

5. According to the research presented in Chapter 6.5, what are the two characteristic parameters of an organic semiconductor that determine the energy landscape and the charge transport mechanism inside of it?

Delocalization degree $\Delta D (= 0–1)$ and variance of Gaussian distribution $\Delta E = \sigma$.

6. How can one determine experimentally if the dominant charge transport regime in an organic semiconductor is coherent or incoherent?

By measuring the mobility at different temperatures. If the logarithm of the mobility increases with the inverse of the temperature, then the charge transport regime is coherent. If it decreases, it is incoherent.

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