Nanostructural properties 2009/10

Mini-course on fundamental electronic and optical properties of organic semiconductors (part 2)

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Outline

➔ A. Introduction and Electronic Properties

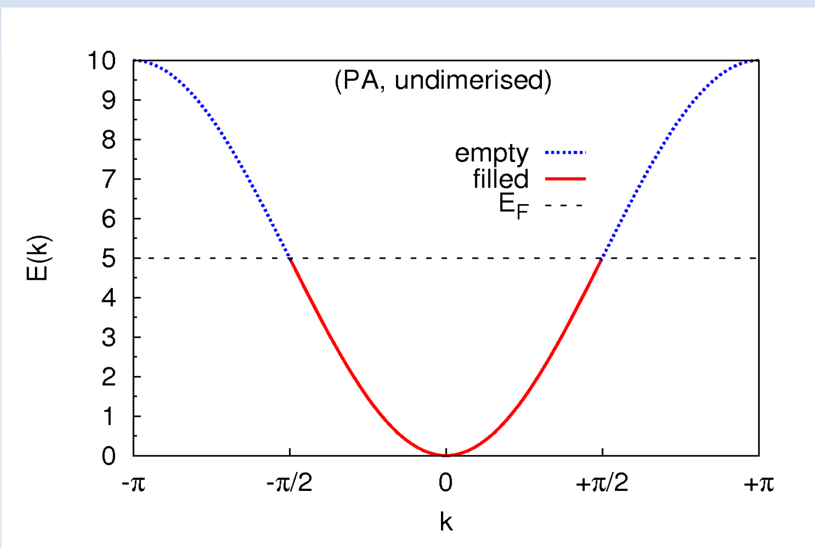
1. A quick overview of organic electronics and a few key concepts
2. A summary of semiconductor physics
3. Organic electronics vs Silicon electronics
4. Light-Emitting Devices and Solar Cells
5. Challenges and open problems

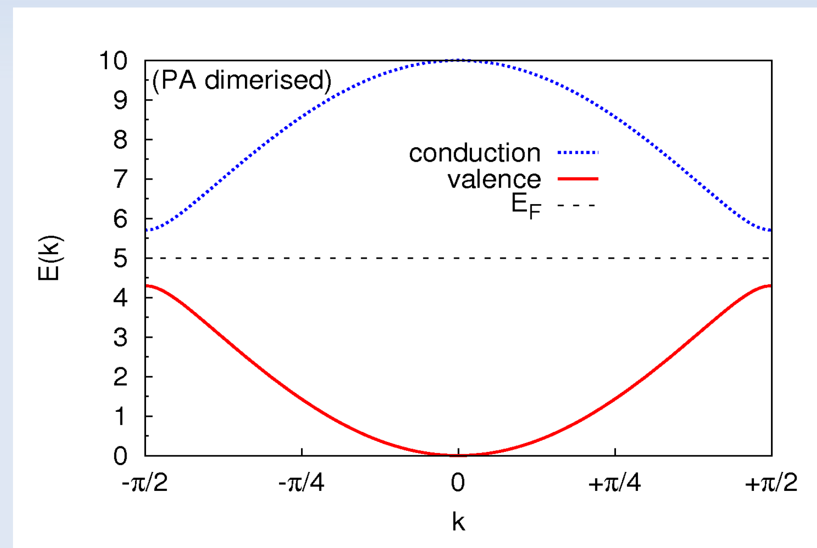
Worked example: band structure of polyacetylene

➔ B. Optical properties

PA Band Structure (see Notes)

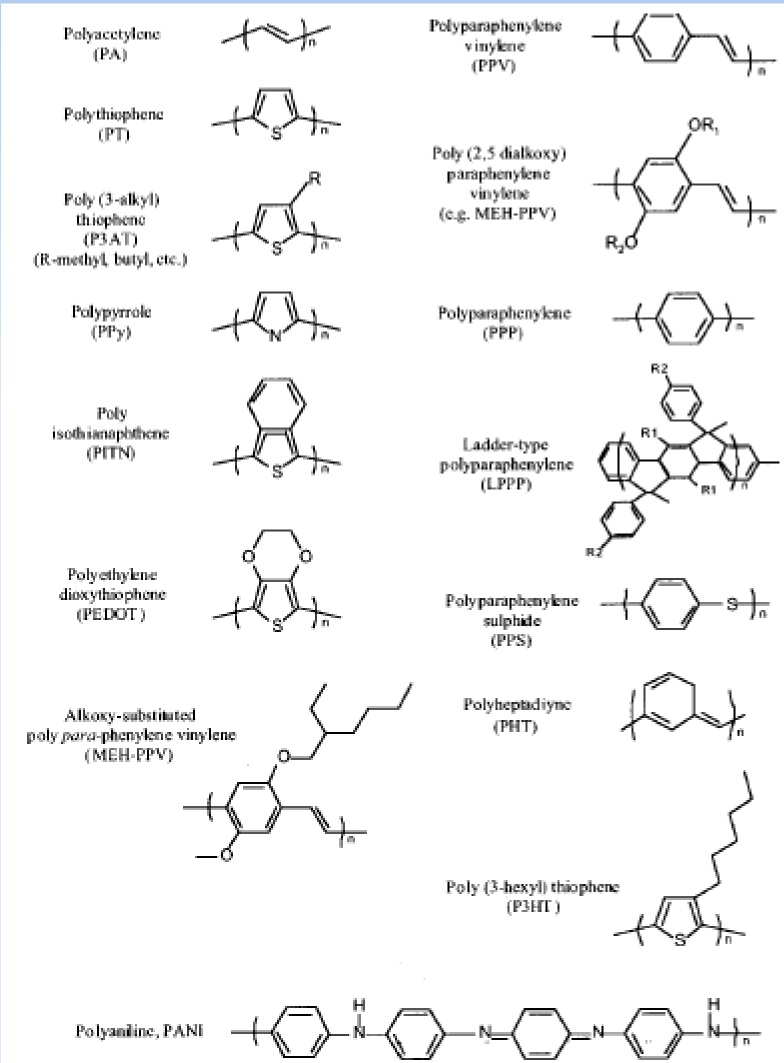
Metal or Semiconductor?
It depends on the structure!





<u>Homework:</u> Work out the dimerised case

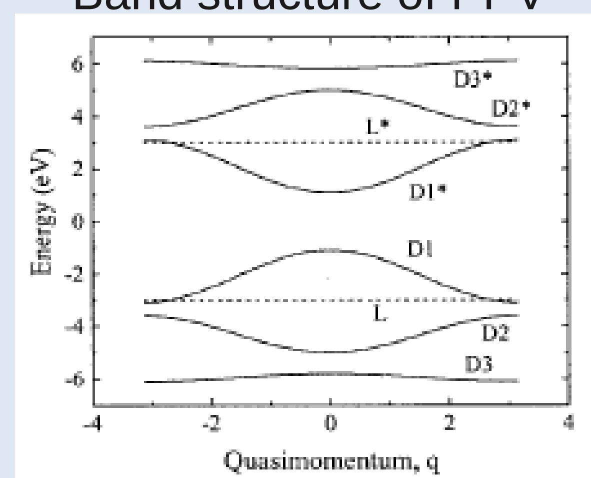
π-Conjugated Polymers



<u>Main features</u>: **bond alternation → electronic delocalisation of π-electrons**

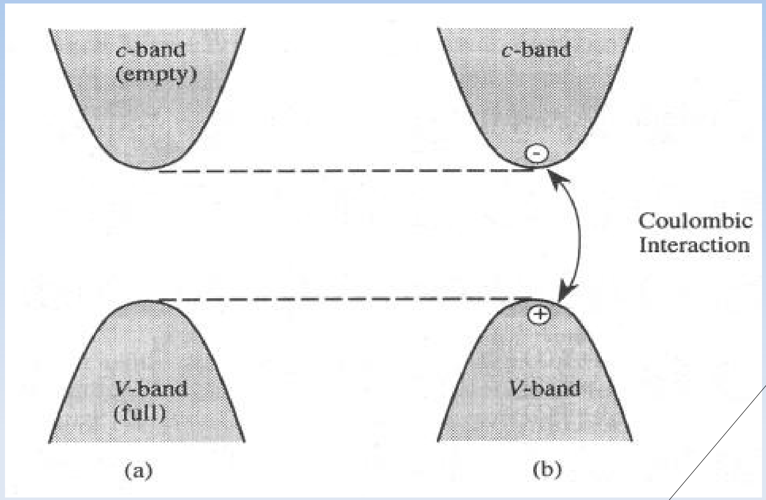
Change molecular structure and chemistry to tailor electron properties

Band structure of PPV



Heeger, Rev.Mod.Phys (2000)

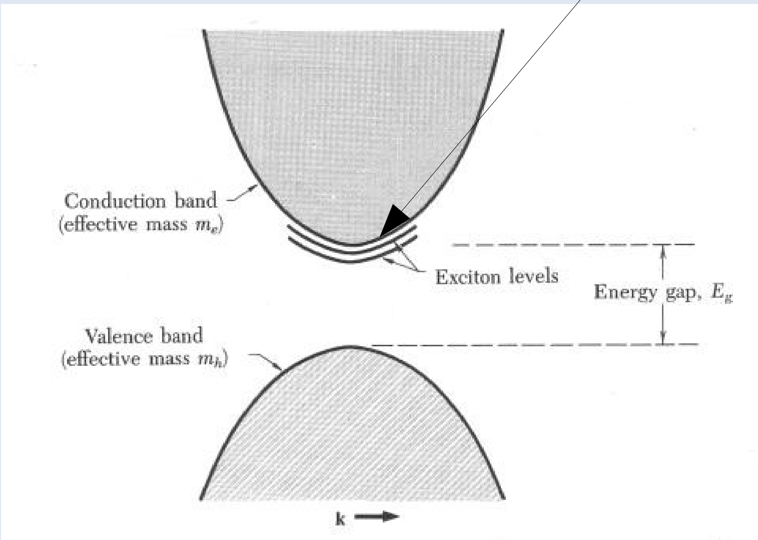
Excitons



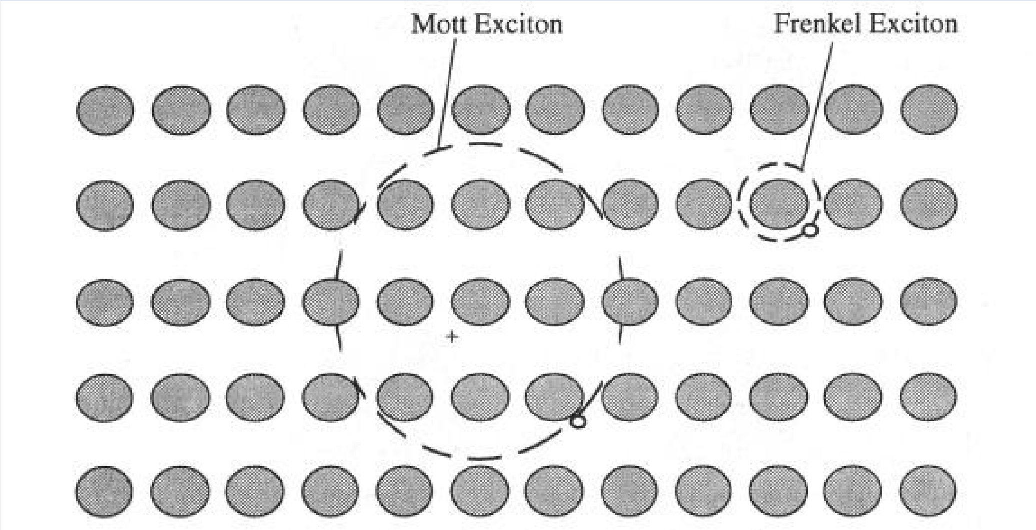
We neglected the electron-hole interaction (Coulomb)

Example: H atom

$$E_n = -\frac{m_{eff} e^4}{2(4\pi\epsilon_0\epsilon_r)^2 \hbar^2 n^2}$$



Two types of exciton: weakly bound (Wannier-Mott) and strongly bound (Frenkel)



From:http://kottan-labs.bgsu.edu/

Excitons

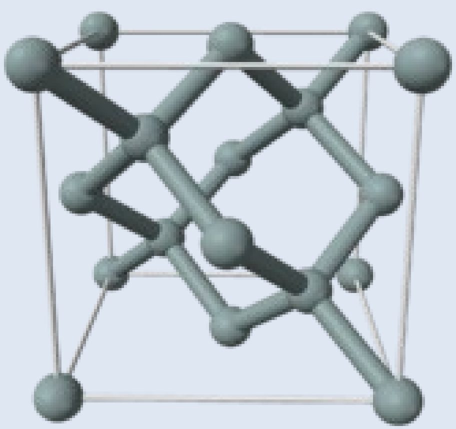
Energetic consideration:

- **Thermal energy(300K) ~0.025 eV**
- **Wannier-Mott excitons ~0.1 eV**
- **Frenkel excitons ~1.0 eV**

[1 eV/part = 23 kcal/mol]

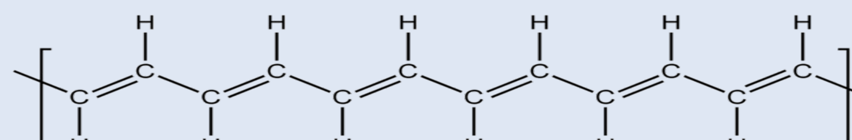
Message: it's hard to dissociate Frenkel excitons at room temperature! Interfaces needed

Si



Wannier-Mott

PA

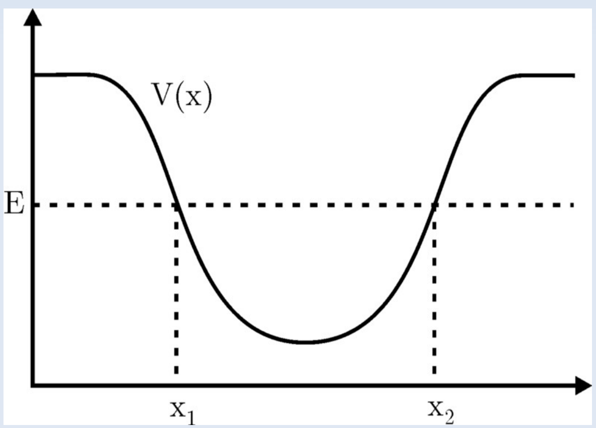


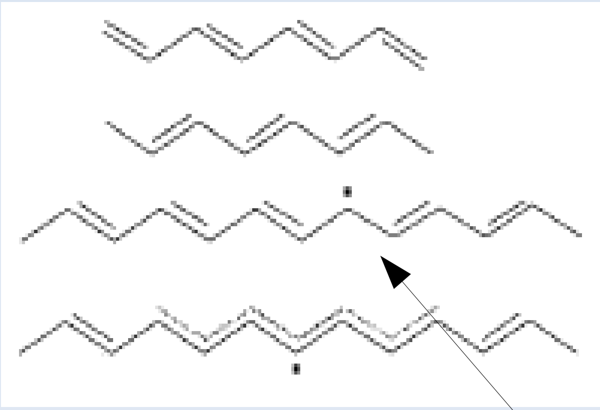
Frenkel

WHY? Electronic screening (ε_r) is more effective in 3D

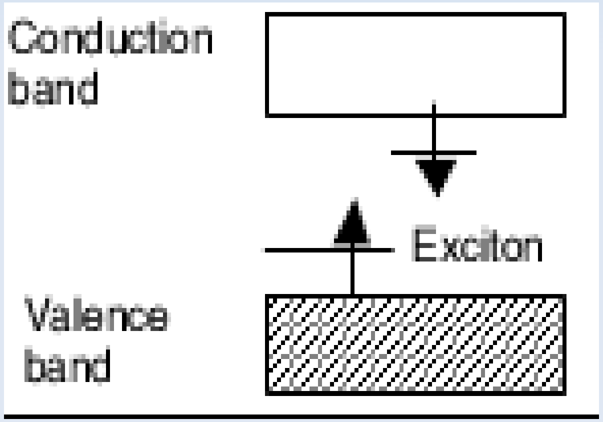
Polymer Chain Deformations

Polymer chains can deform about an electron-hole pair, <u>polaron-exciton</u>

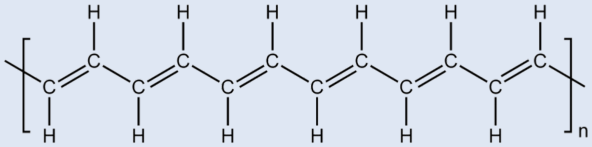




Heeger, Rev.Mod.Phys (2000)



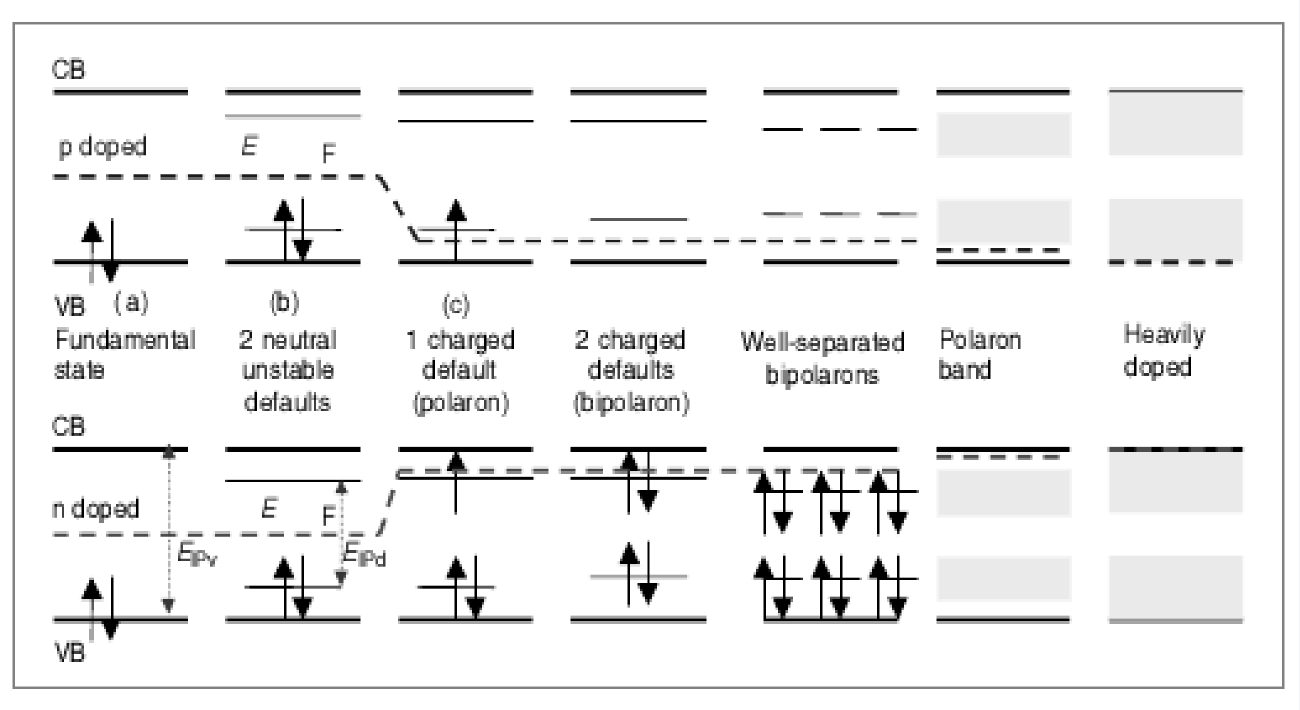
Moliton&Hiorns
Polym. Int. (2004)



<u>Local deformation</u>, like a defect or an impurity level (localised state)

Doping

- Charge transfer
- Field effect
- Carrier injection
- Optical doping
- Acid-basic



Moliton&Hiorns Polym. Int. (2004)

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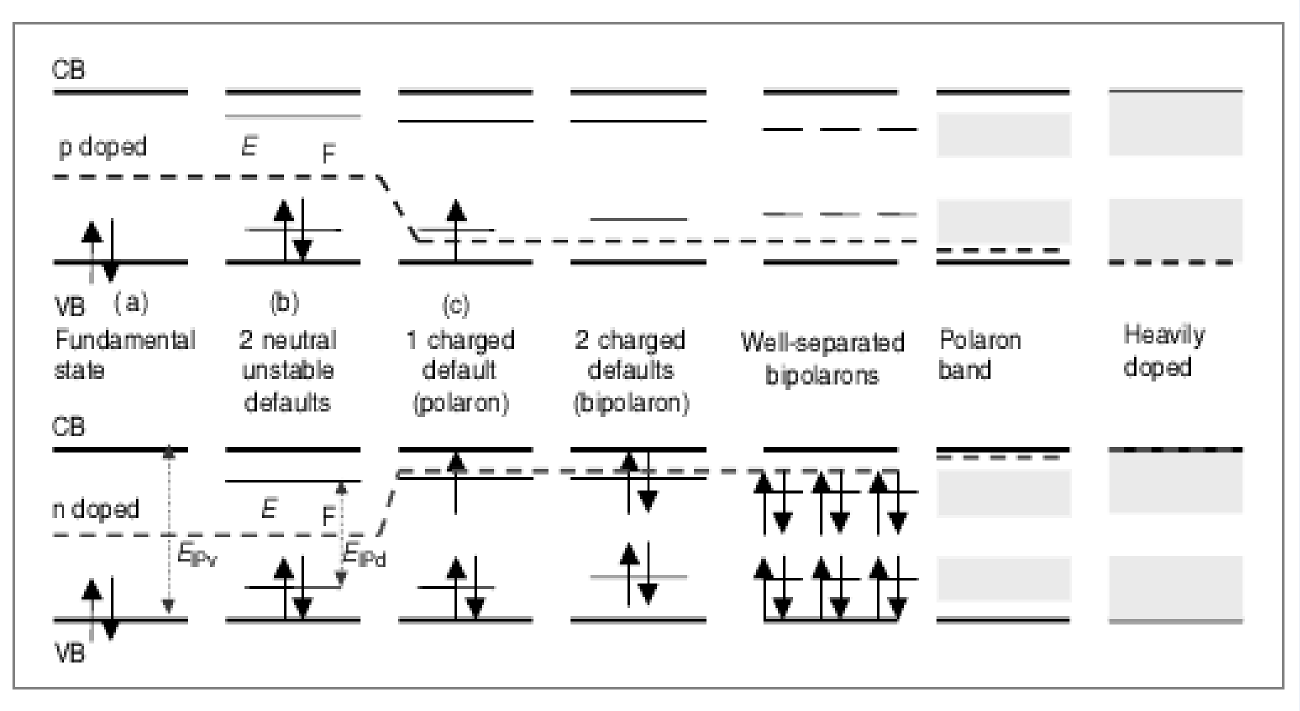

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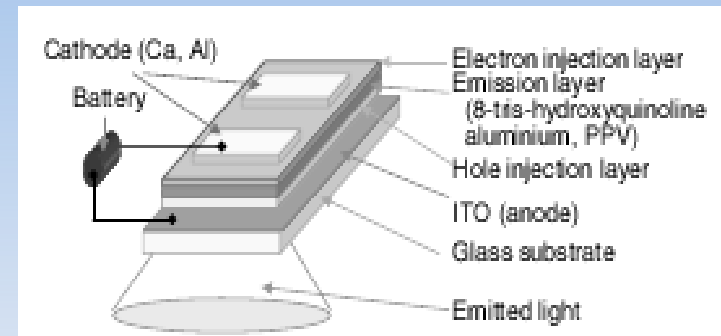
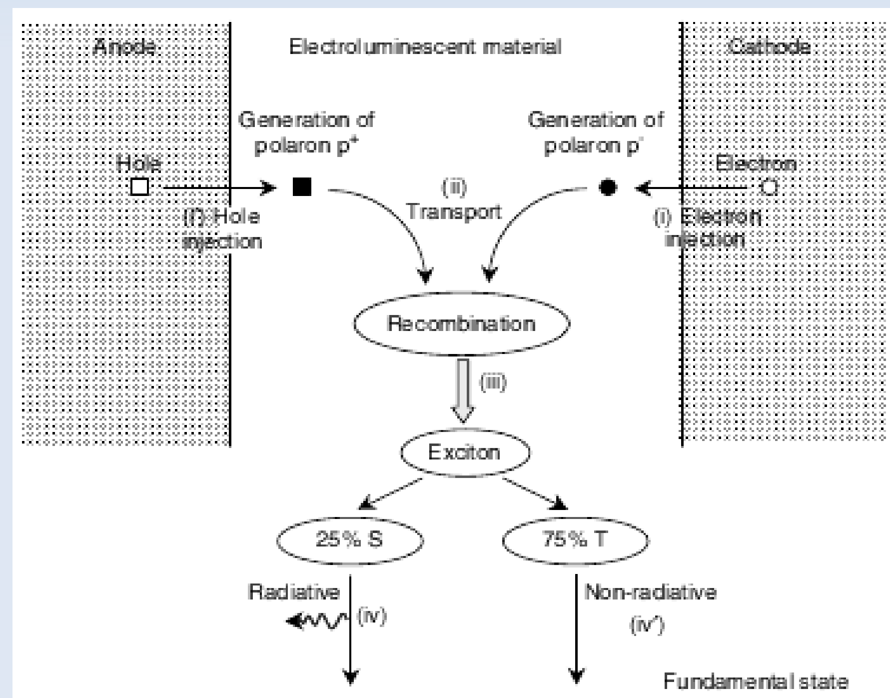
Light-Emitting Devices (LEDs)



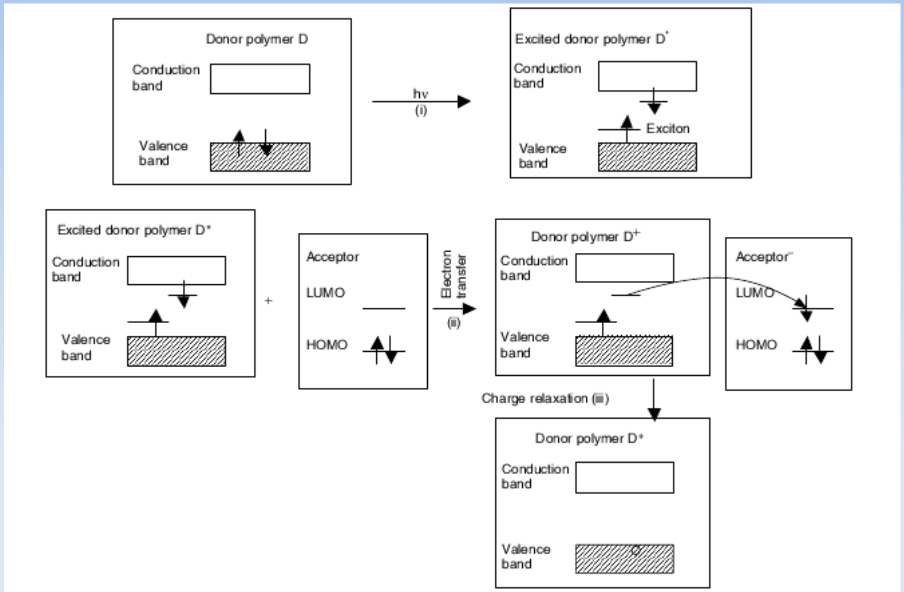
Low mobility is advantageous

Big issue: polymer degradation (Blue OLEDs)



Moliton&Hiorns Polym. Int. (2004)

Solar Cells



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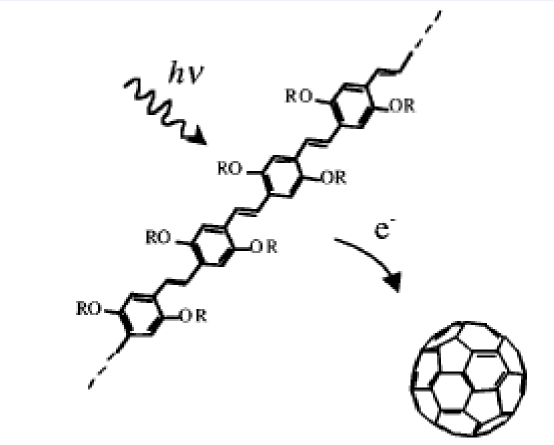
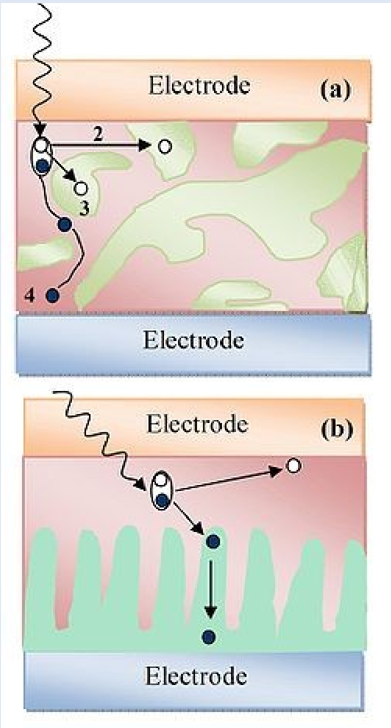
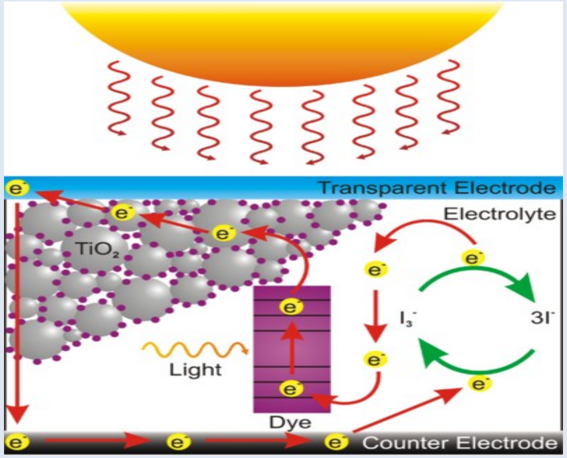


Competition between exciton relaxation and dissociation times

Low efficiency ~3%





Dye-sensitized solar cell (Grätzel)