Organic light-emitting diodes

Chemical and electronic Structure of organic materials

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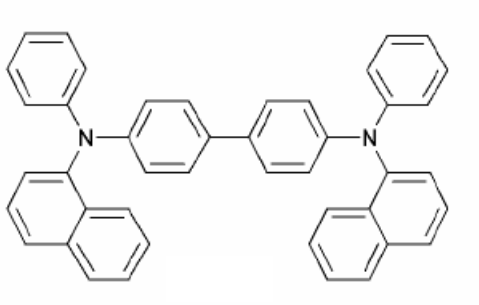
Organic Materials

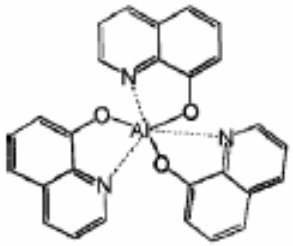
C 、H、O、N、S.....



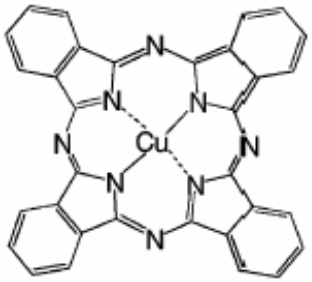
α-NPD

Organic metallics

Alq_3、CuPc.....

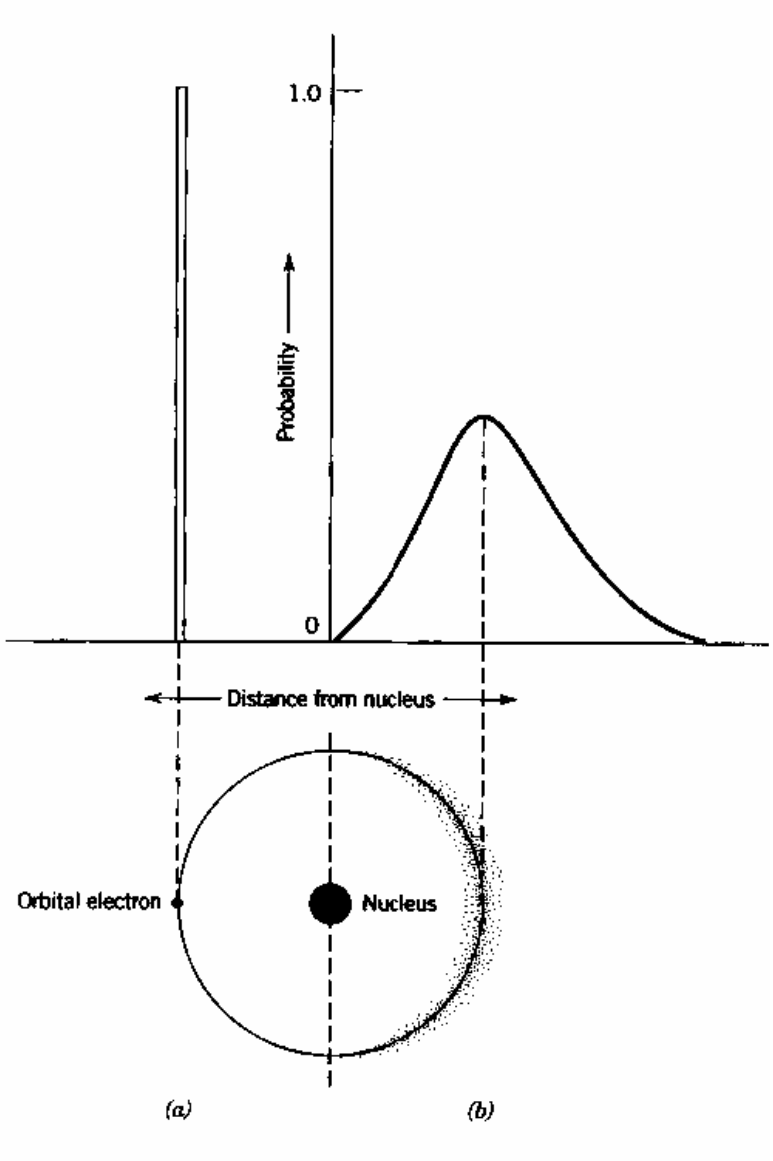


Alq_3

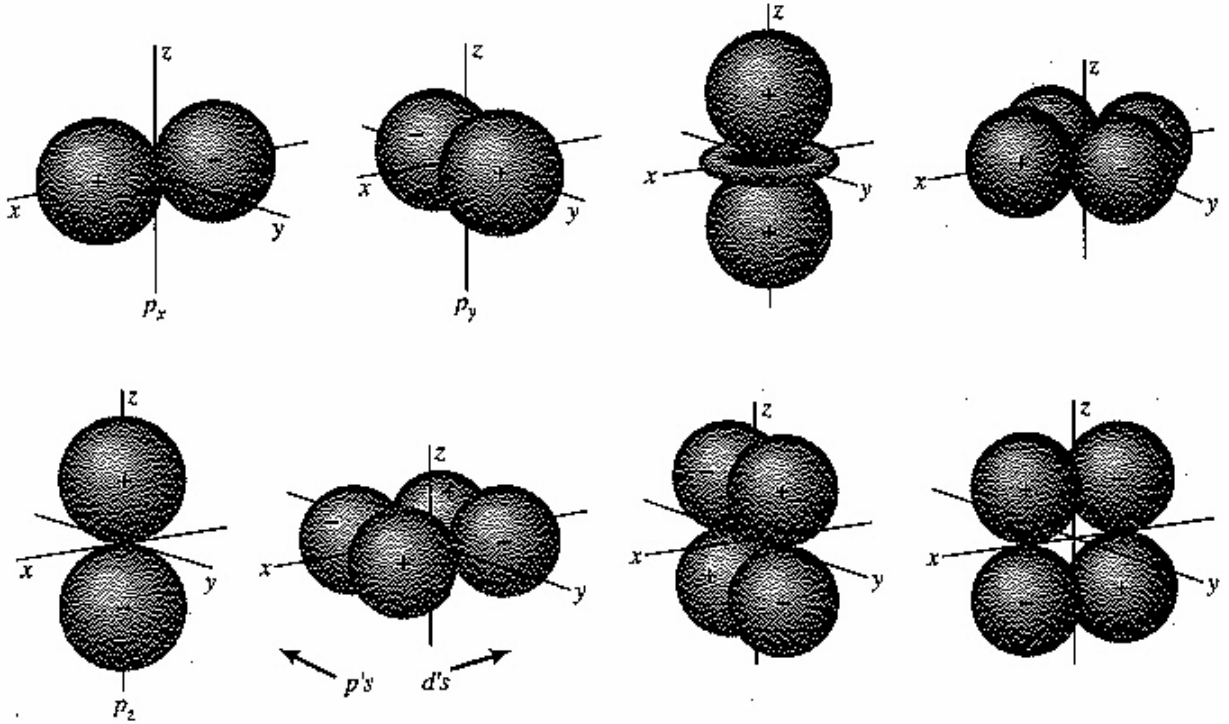


CuPc

Comparison of Bohr and wave-mechanical atom models



Atomic Orbitals



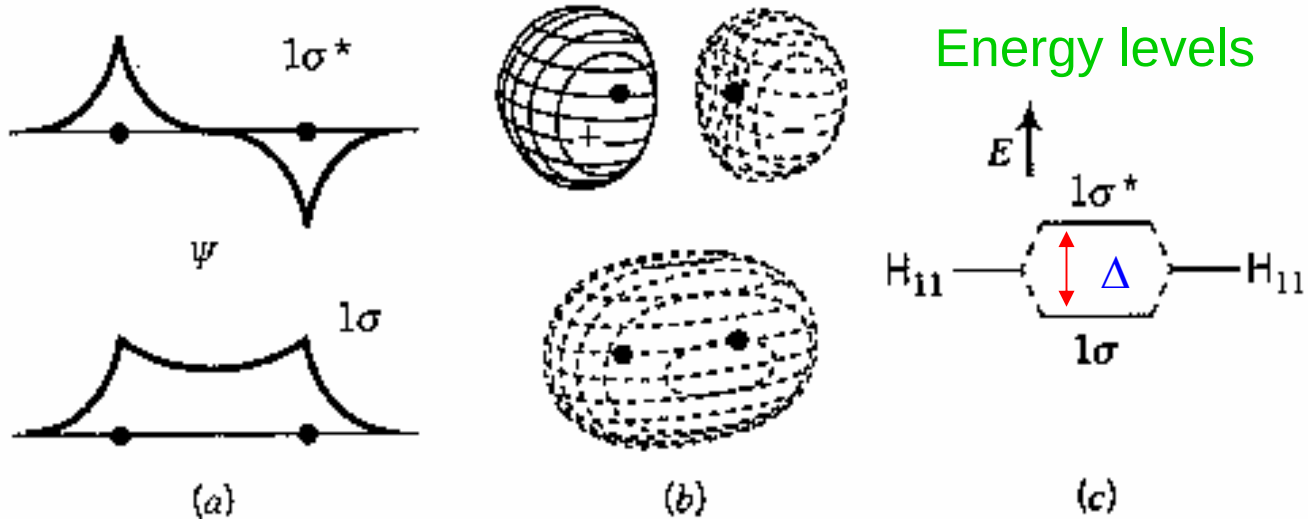
φ : one-electron wave function

φ^2 : electron density

Molecular Orbitals

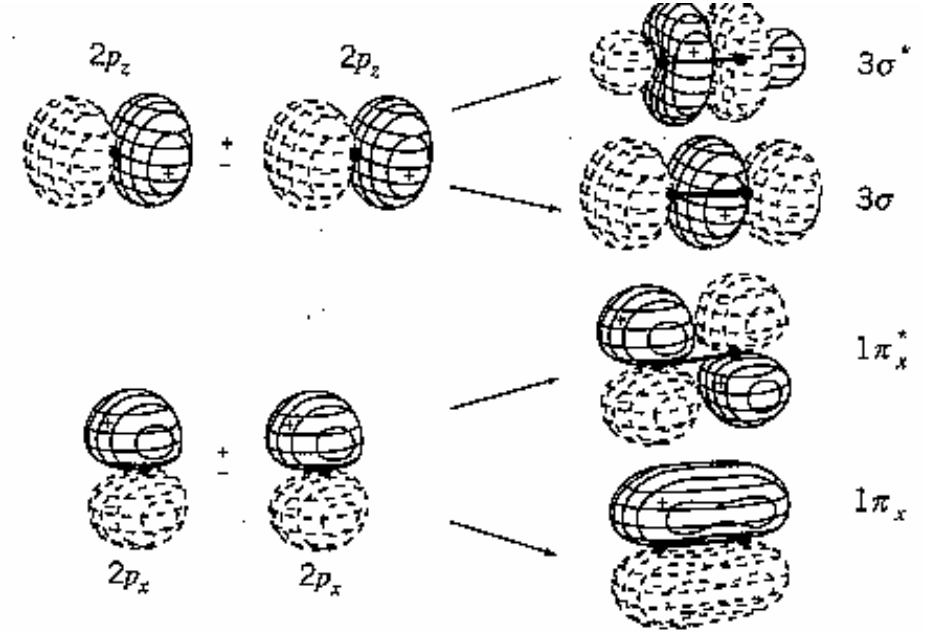
Anti-bonding

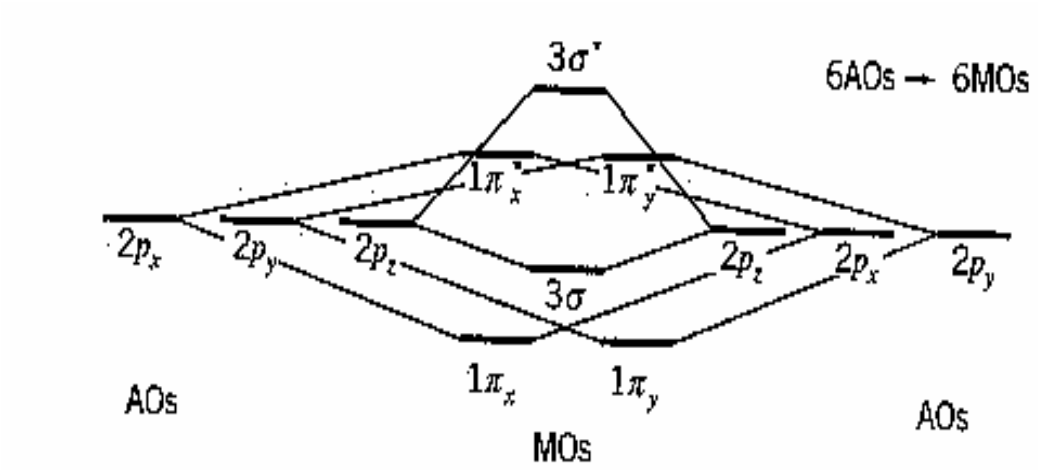
Bonding



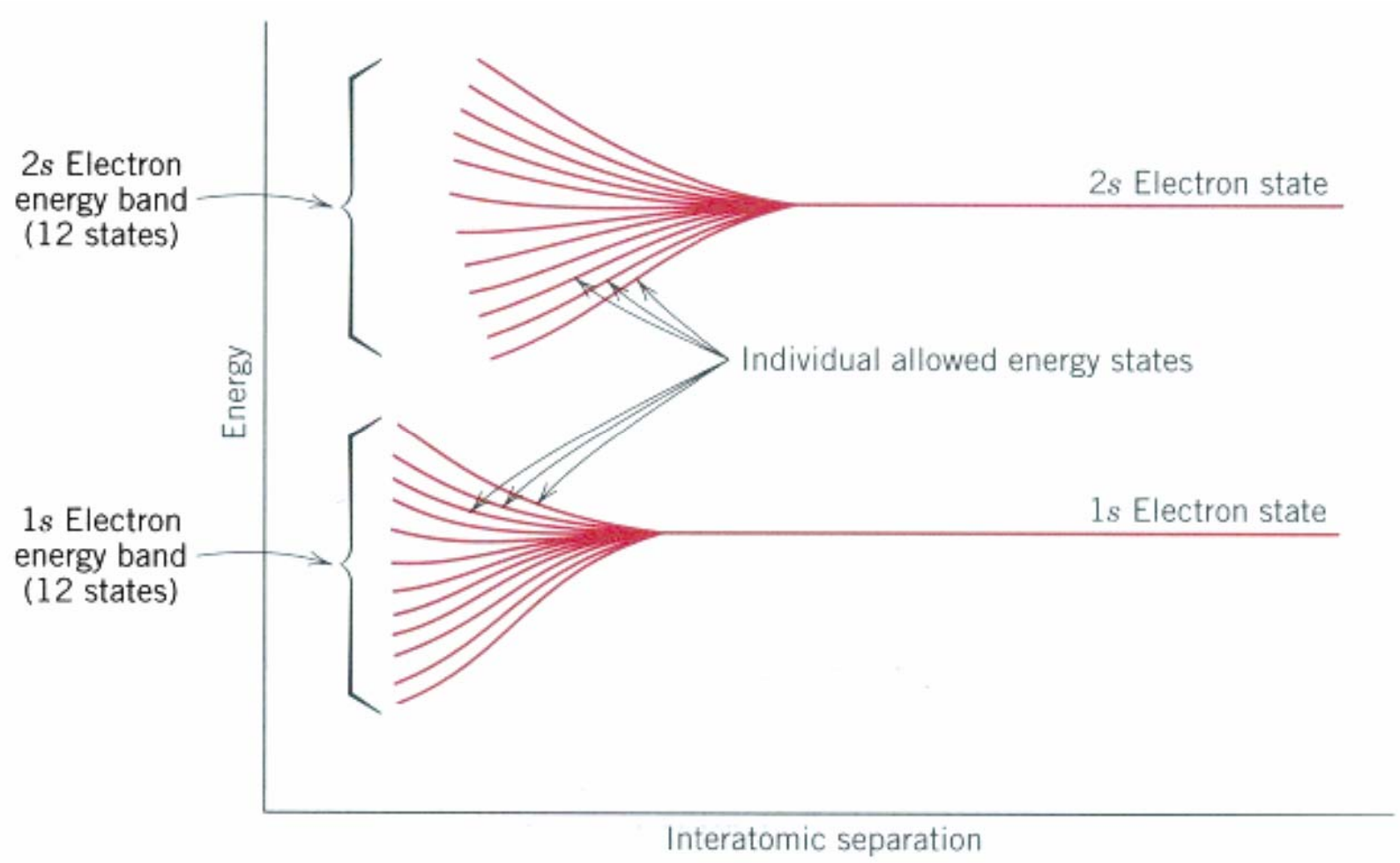
Δ: depends on the degree to which the orbitals occupy the same space or “overlap”

Molecular Orbitals

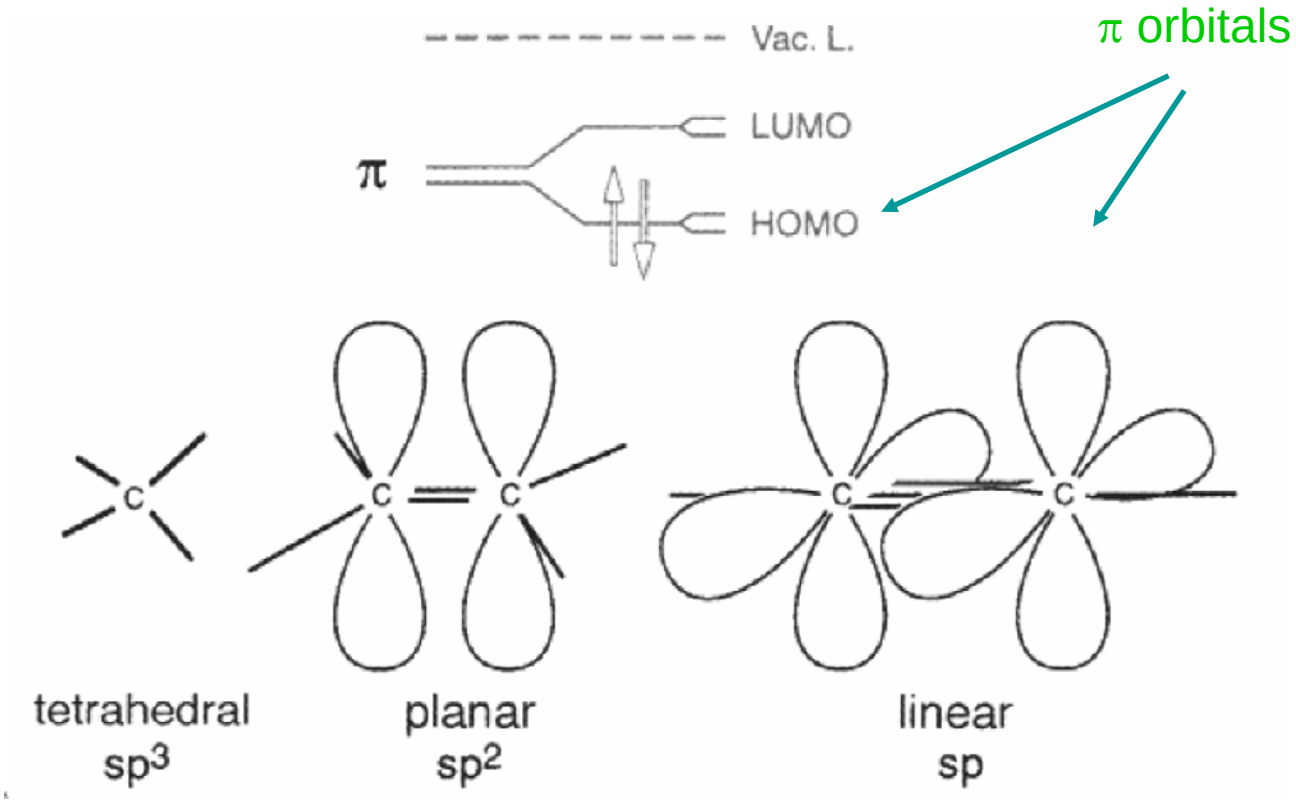




Electronic energy vs interatomic separation of an aggregate of 12 atoms

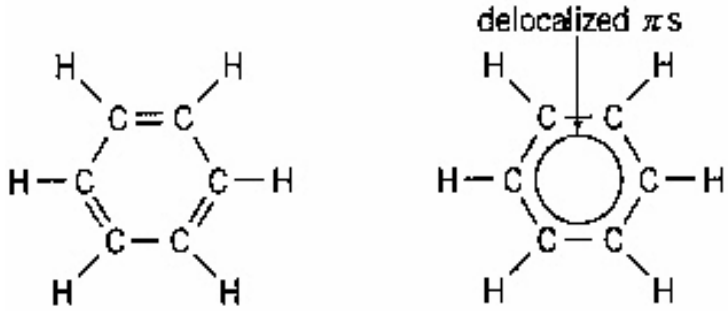


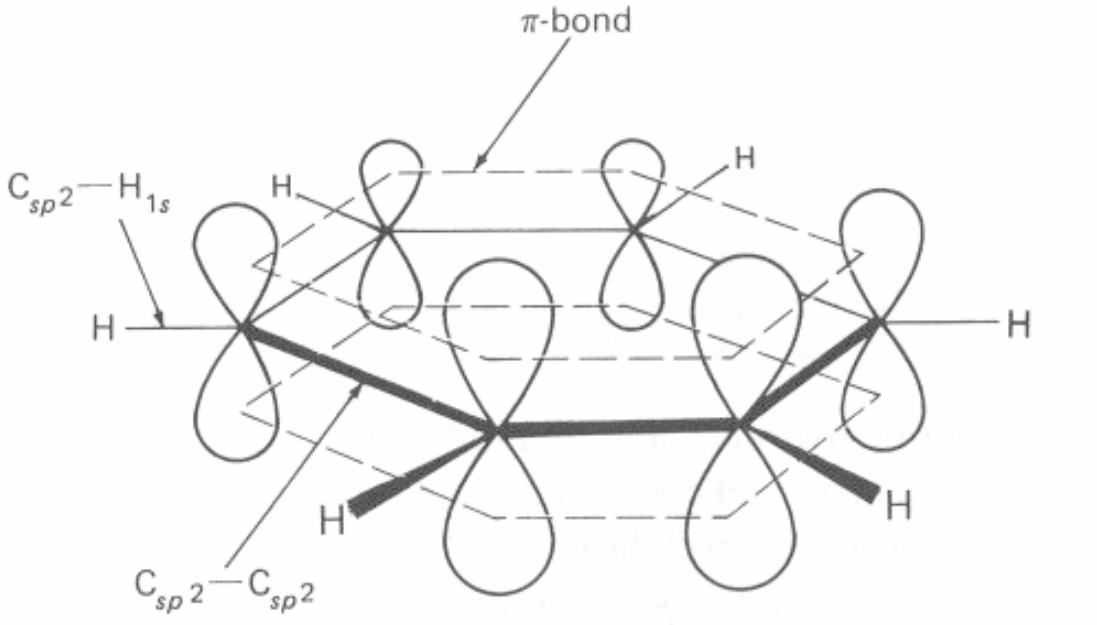
Carbon atom bonding configurations



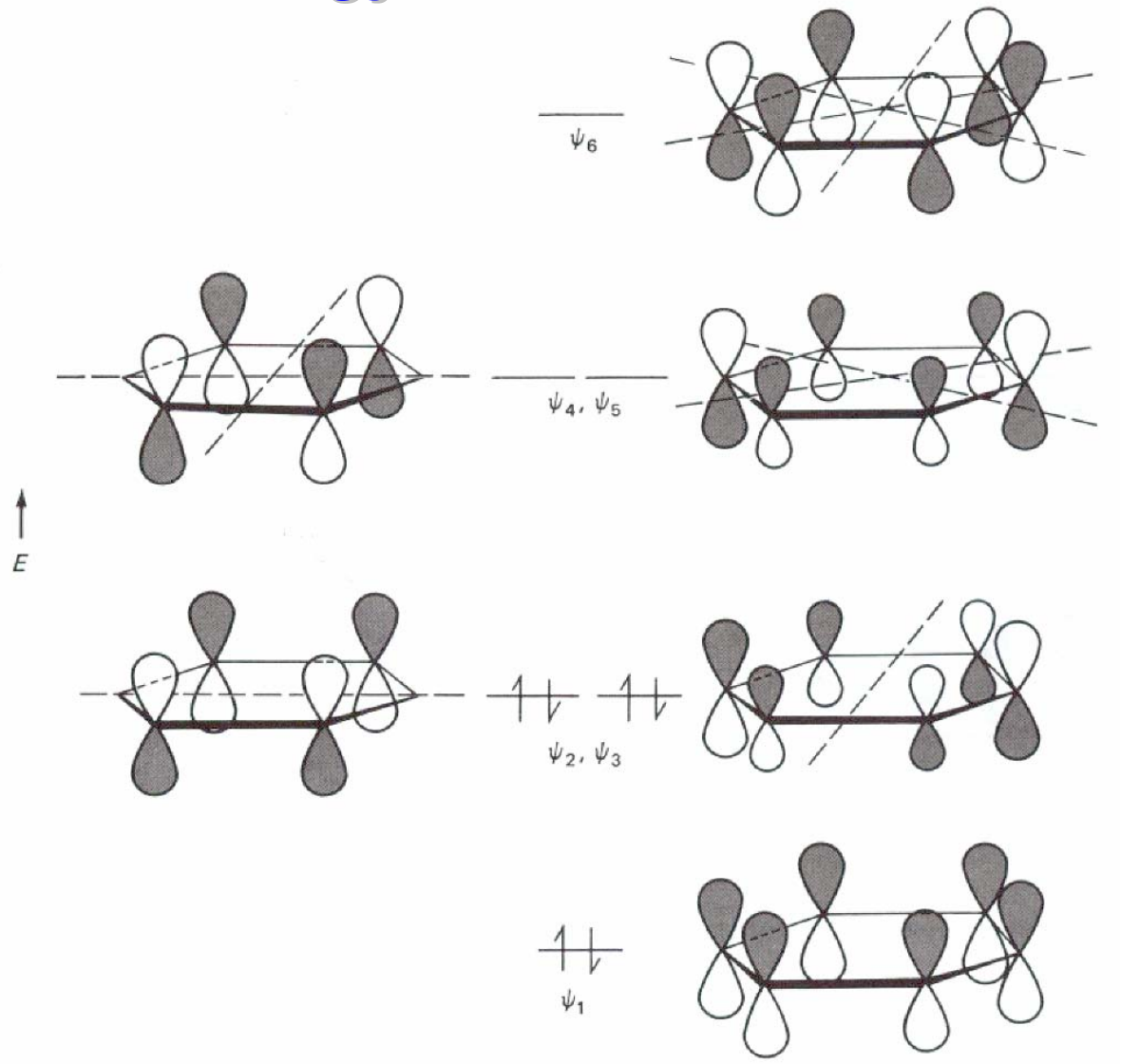
single bond **double bond** **triplet bond**

Orbital structure of benzene (Six Carbons)

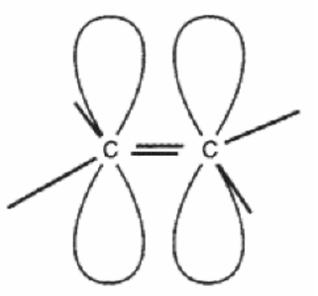


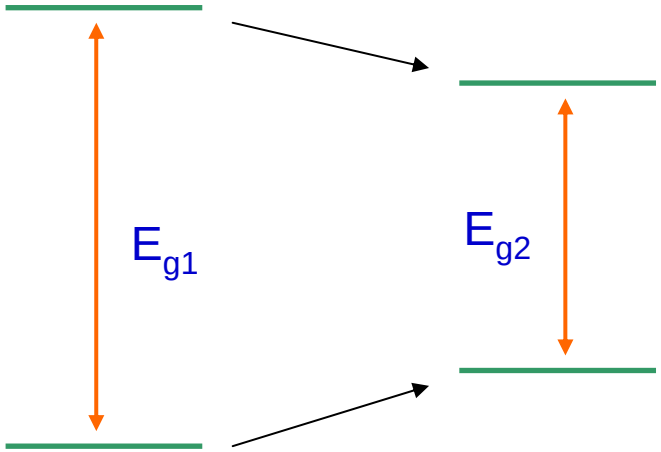


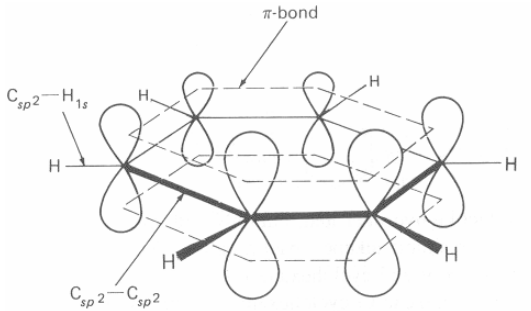
The π-molecular orbitals and energy levels for benzene



Chemical structures of common organic semiconductors







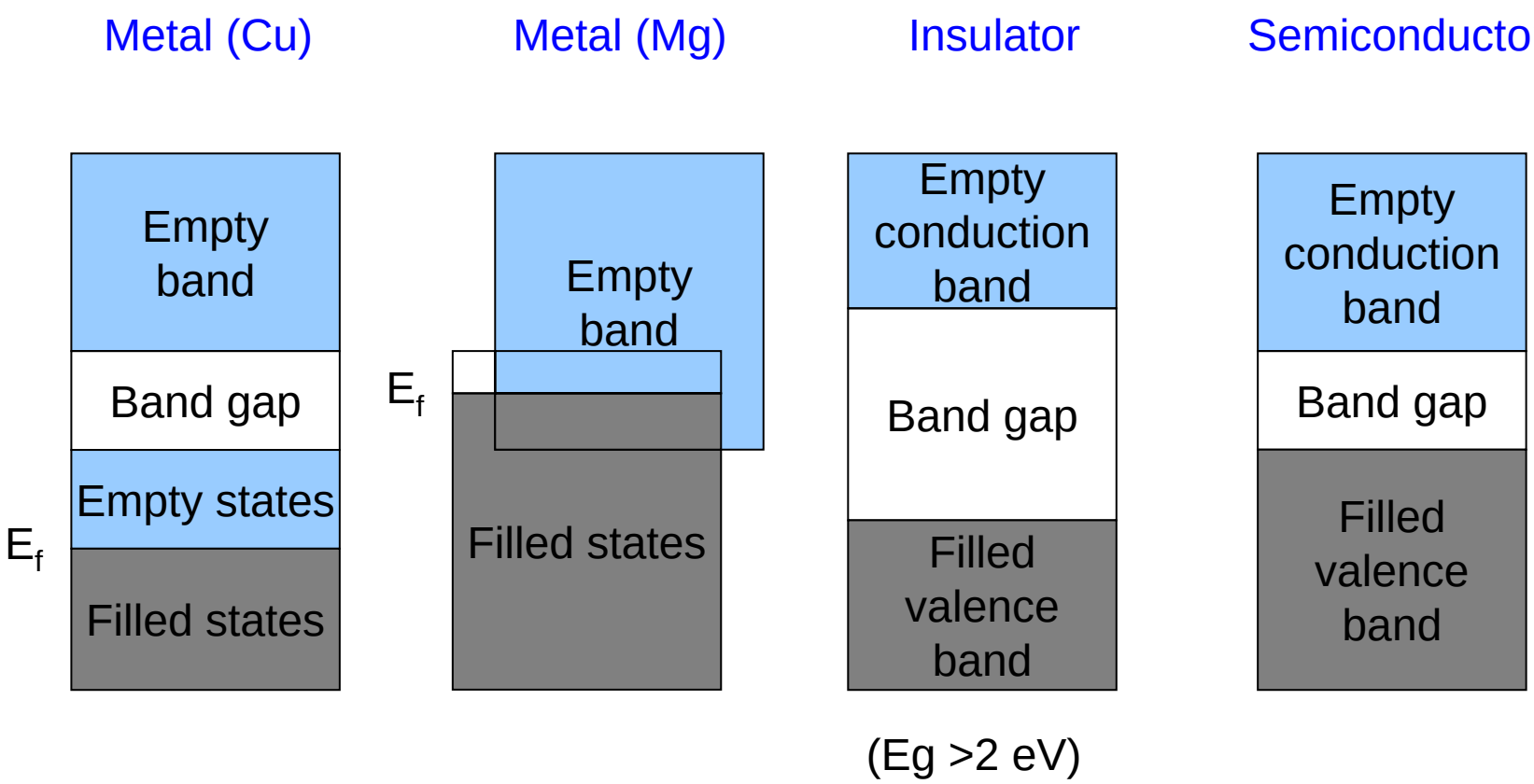
The lowest electronic transition (band gap, E_g)

Ethylene (C_2H_4) : E_{g1} = 6.9 eV

Benzene (C_6H_6) : E_{g2} = 4.6 eV

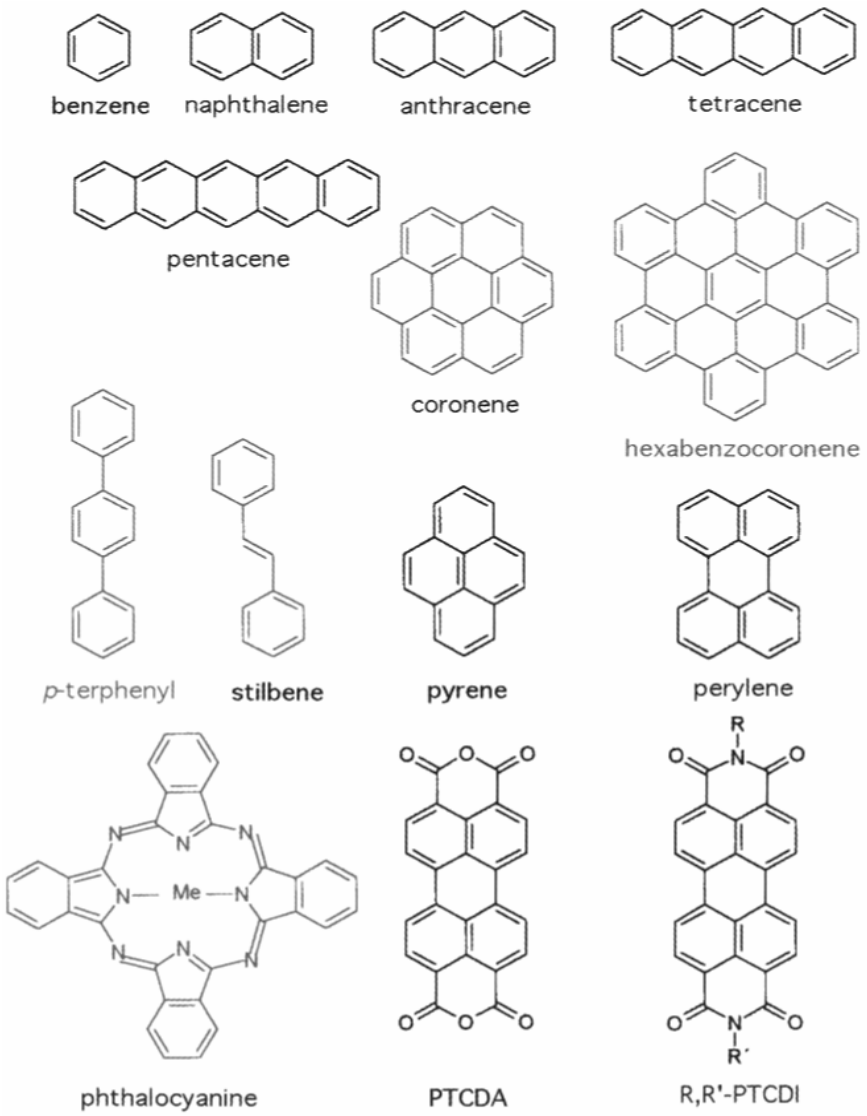
More delocalized π electrons, the lower the band gap energy

Electron band structures in solids at 0 K

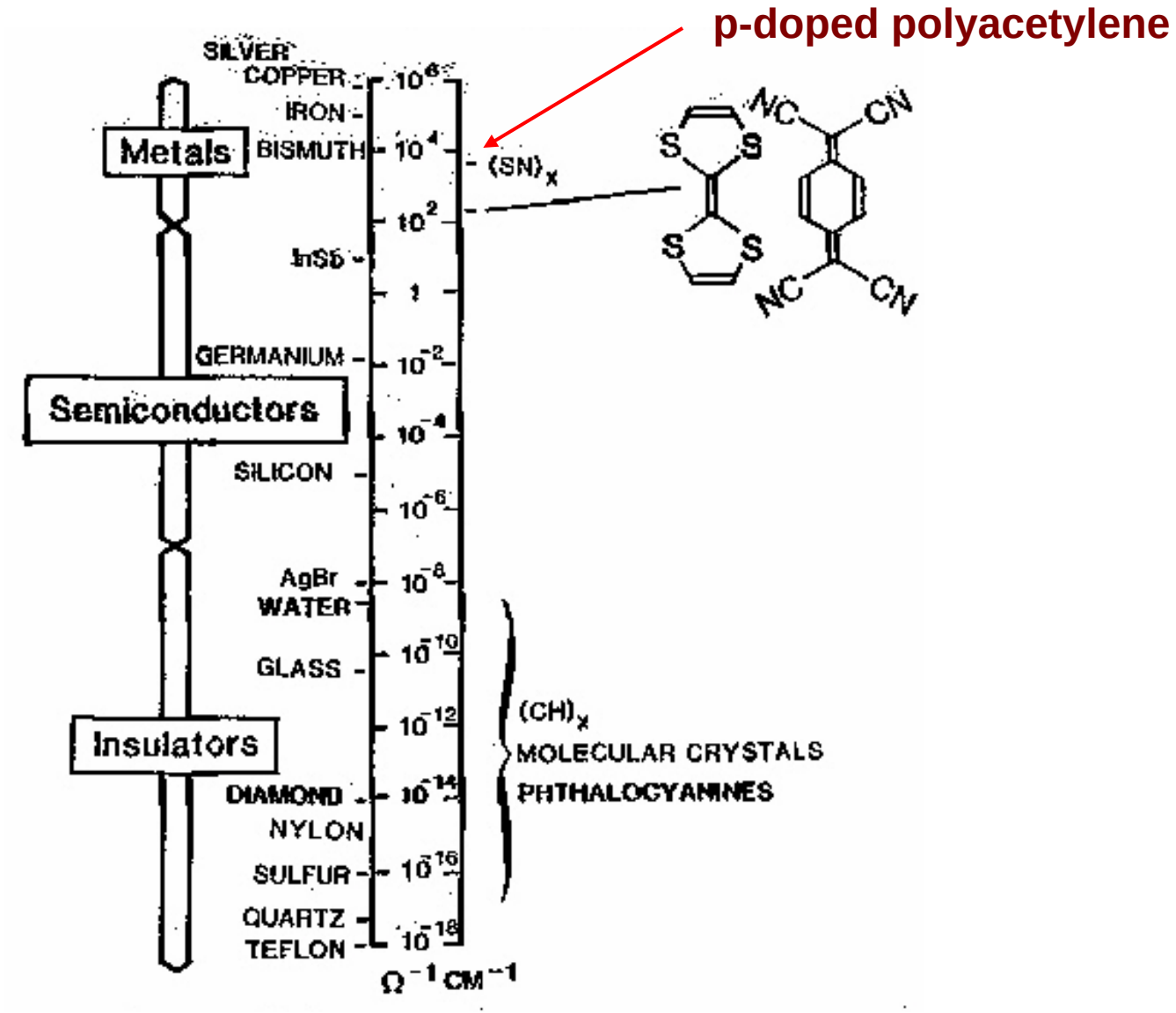


$10^{7}\ \Omega^{-1}\ cm^{-1}$ **10^{-10} - $10^{-20}\ \Omega^{-1}\ cm^{-1}$** **$10^{-6}$ - $10^{4}\ \Omega^{-1}\ cm^{-1}$**

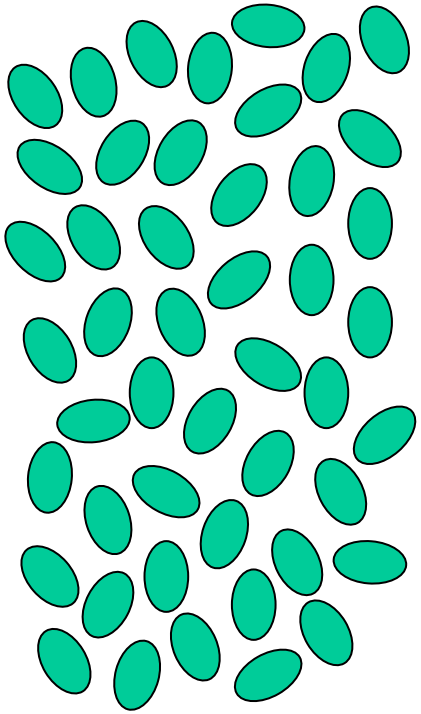
Chemical structures of common organic semiconductors



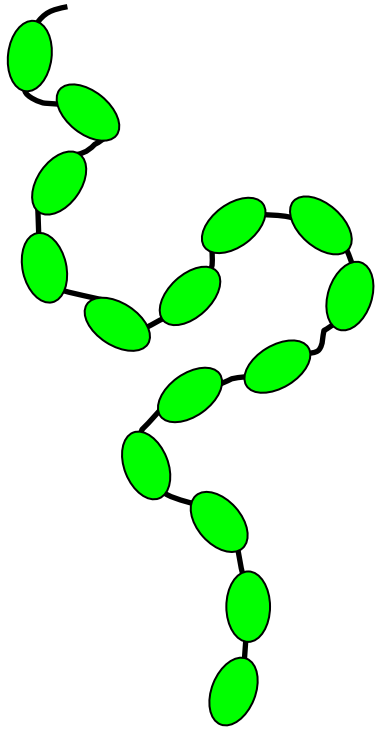
Conductivity domain of metals, semiconductors, and insulators



Organic (Molecular) Semiconductors



Small Molecules



Functional
Polymers

Weak bonding
(van der Waals force)

Low melting point

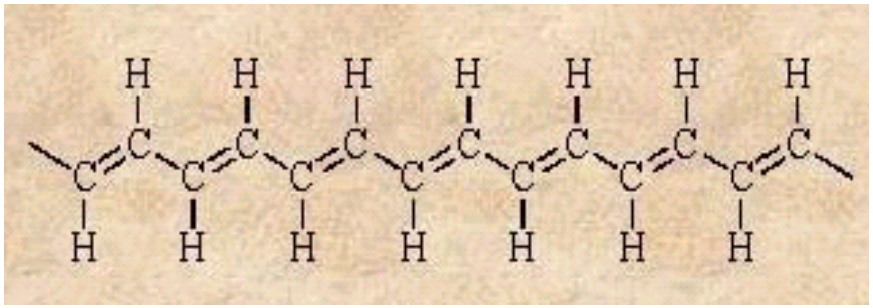
Low conductivity
10^{-8} - 10^{-12} Ω^{-1} cm^{-1}

Conjugation

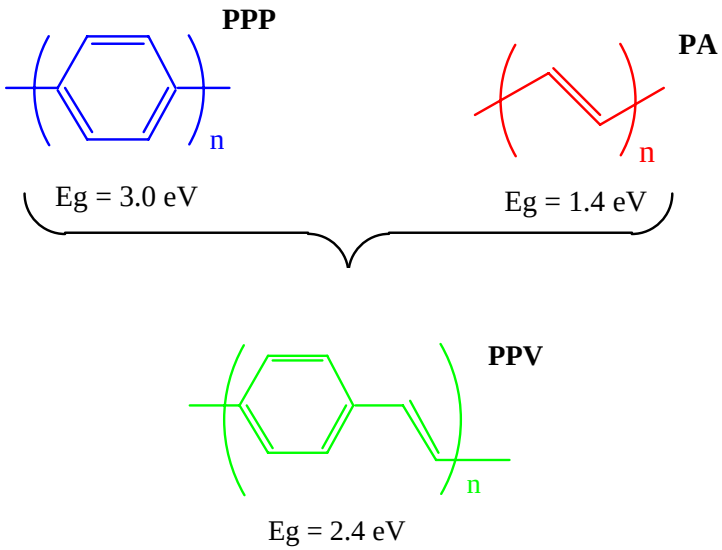
A conjugated system is one having alternating single and double bonds

Conjugated Polymer
Backbones:
alternating single-double bonds

Delocalized π electron clouds



polyacetylene



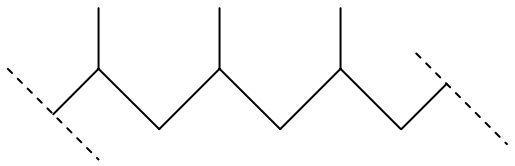
Polymer vs Small Molecular

Polymer, Macromolecules

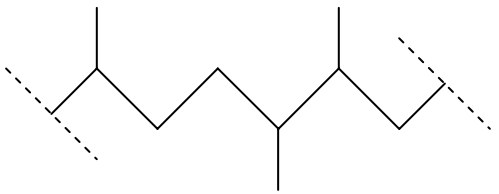
Historically, molecules larger than 10k (10000 g/mole) belong to this group

Technically, all polymers are mixtures

Polymers show isomers, and polymers having the same Chemical formula can show different properties



different



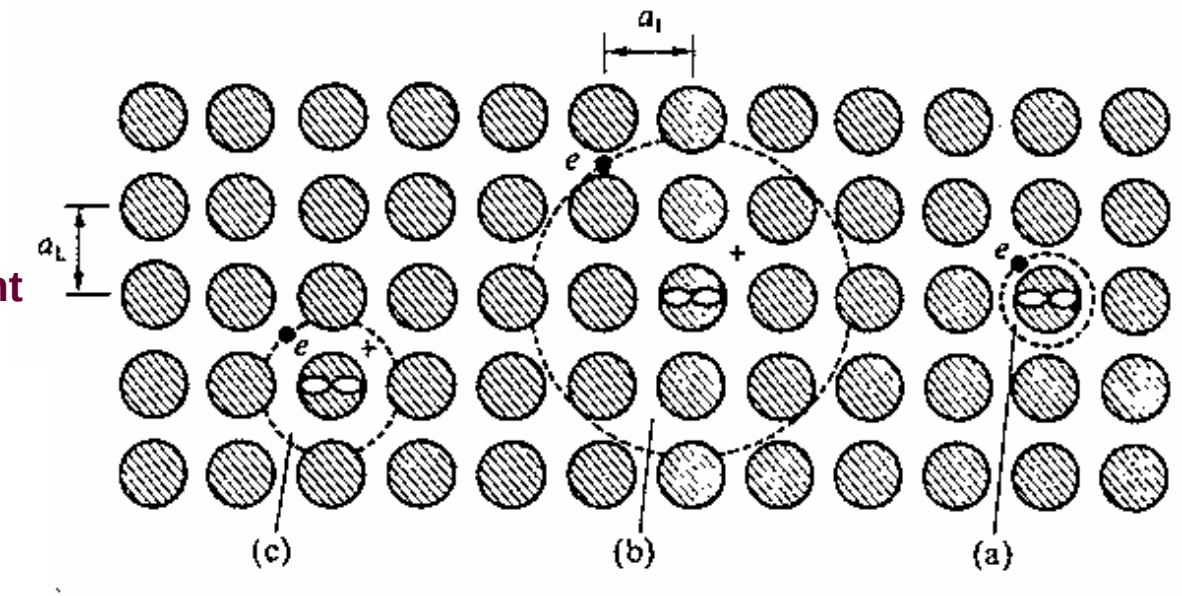
Regioregular - Polypropylene

Random - Polypropylene

Excitons in Organic Materials

Electronic excitation is considered as a quasi-particle, capable of migrating. This is termed as “Exciton”

Excitons can be regarded as bounded electron-hole pairs.
Also can be viewed as the excited states of molecules

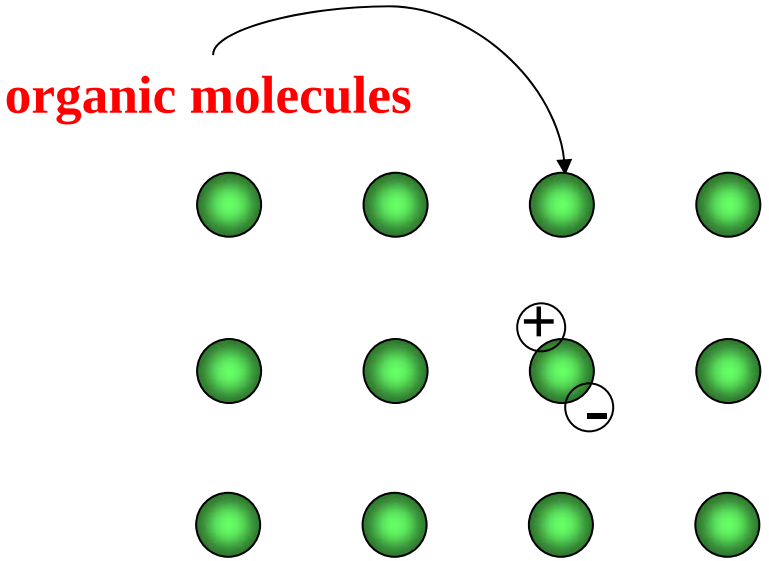


Charge-transfer exciton

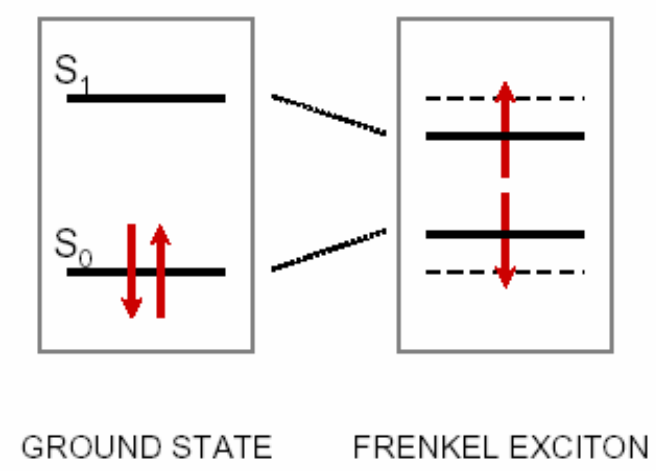
Wannier-Mott exciton

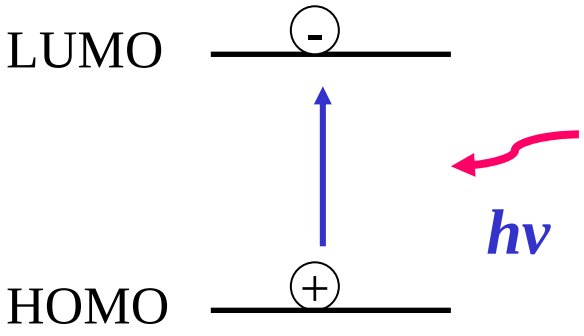
Frenkel exciton

The Nature of Excitons in Organic Materials



Frenkel Exciton





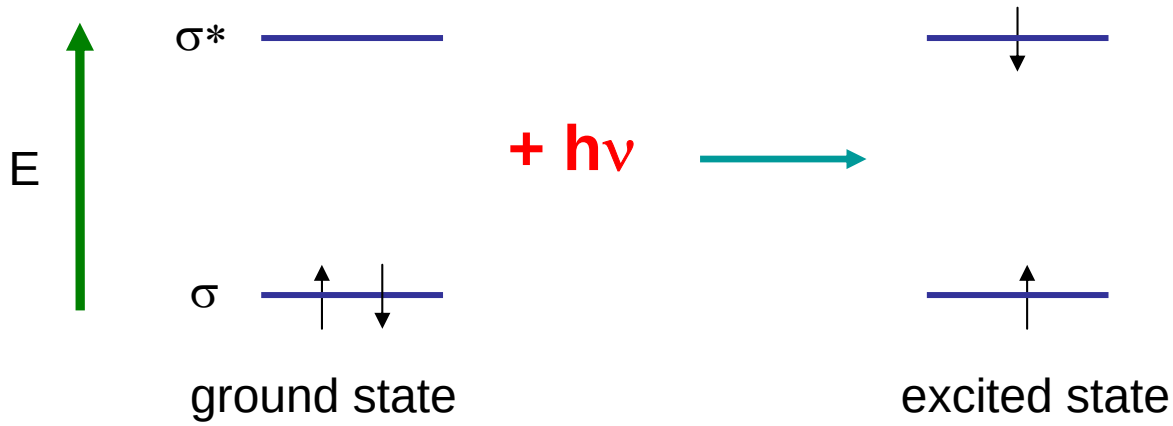
Coulombic interaction

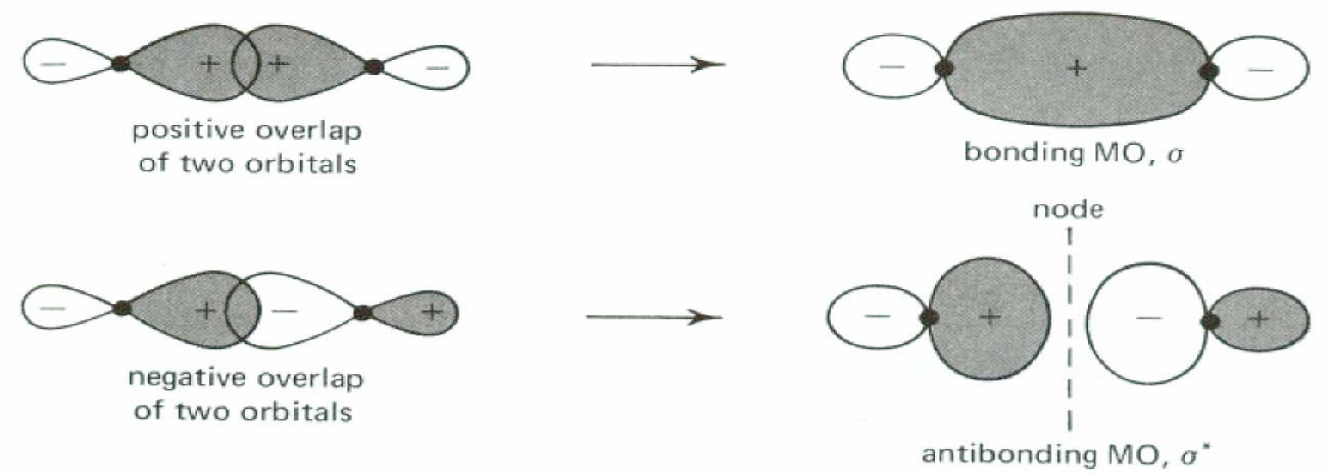
$$E \propto - \frac{q_1 \, q_2}{\varepsilon \, r}$$

(binding energy 0.2 - 1.0 eV

Radius ~ 10Å)

Ultraviolet-visible (UV-vis) Spectroscopy





Ultraviolet-visible (UV-vis) Spectroscopy

λ ~ 150 nm, $\sigma - \sigma^*$ transition

λ < 200 nm, vacuum ultraviolet, strongly absorbed by the oxygen

λ = 200 - 400 nm, ultraviolet,
λ = 400 - 750 nm, visible,
} $\pi - \pi^*$ transition

$\pi - \pi^*$ transitions

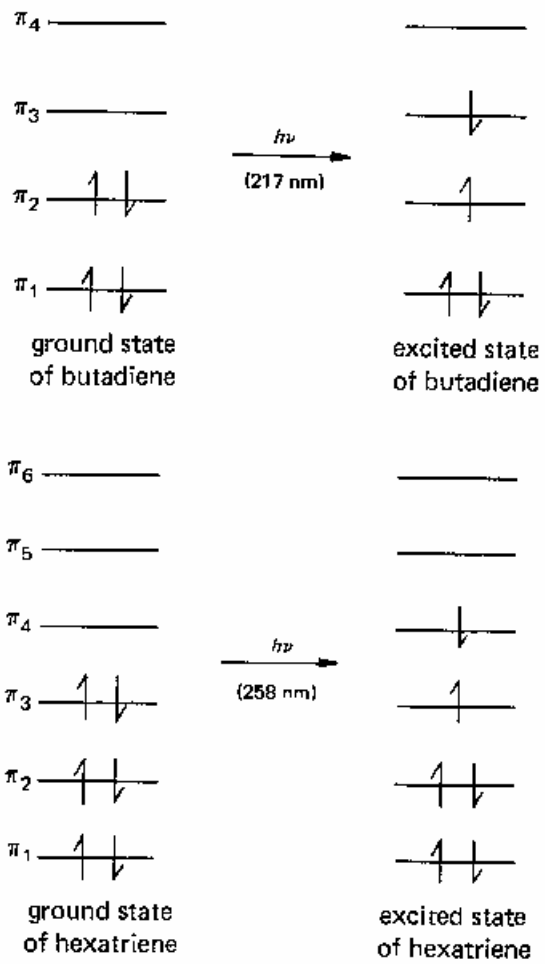
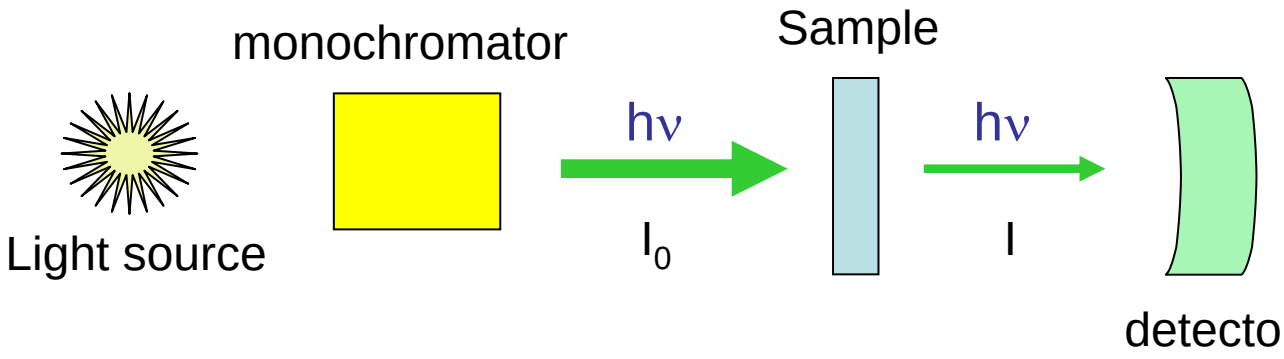


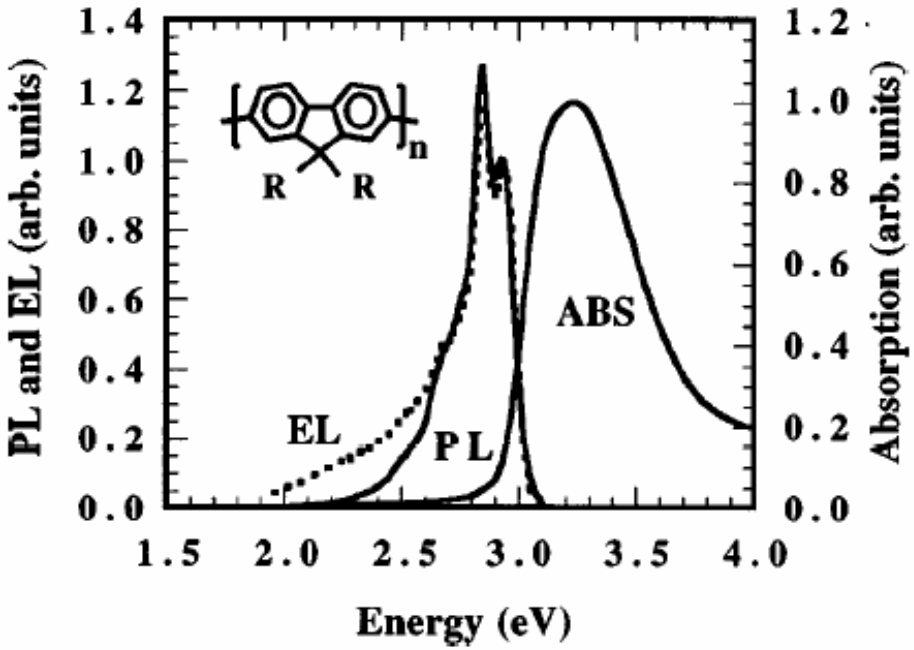
FIGURE 22.23 Electronic excitation of butadiene, $CH_2{=}CH{-}CH{=}CH_2$, and 1,3,5-hexatriene, $CH_2{=}CH{-}CH{=}CH{-}CH{=}CH_2$.

The longer the chain of conjugation
The longer the wavelength of the absorption band

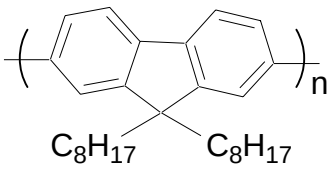
Ultraviolet-visible (UV-vis) Spectroscopy



$$A = - \log \left(\frac{I}{I_0} \right)$$

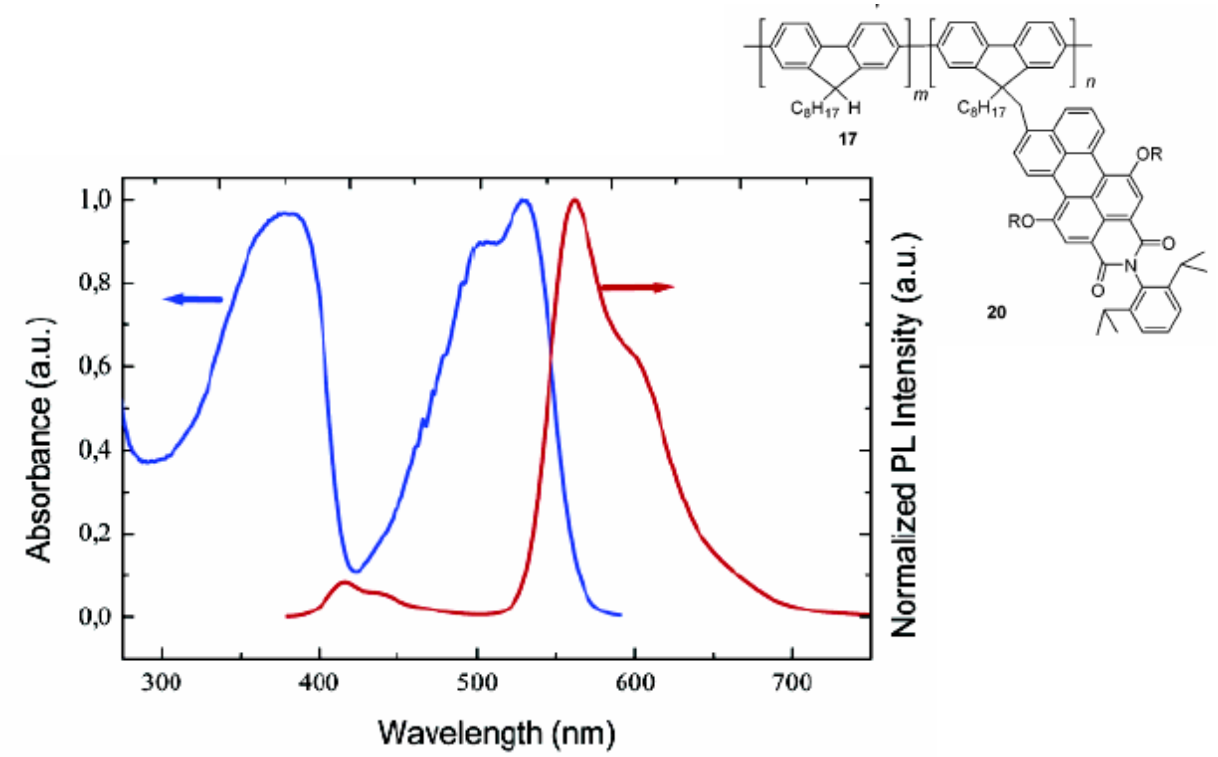


UV-vis Spectroscopy of polyfluorene

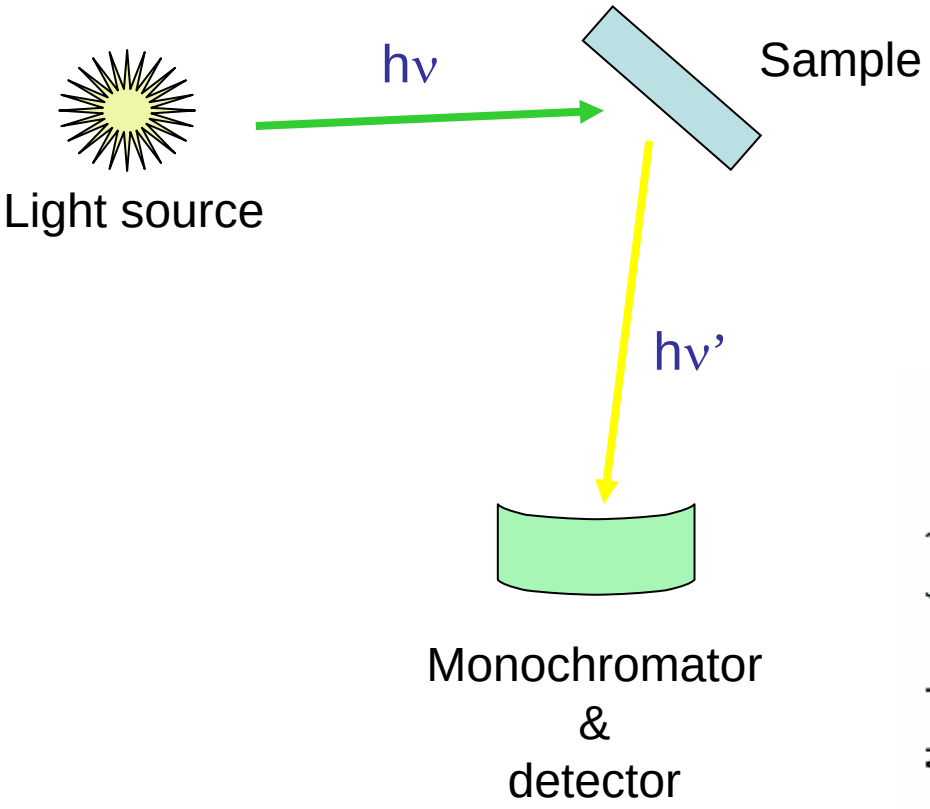


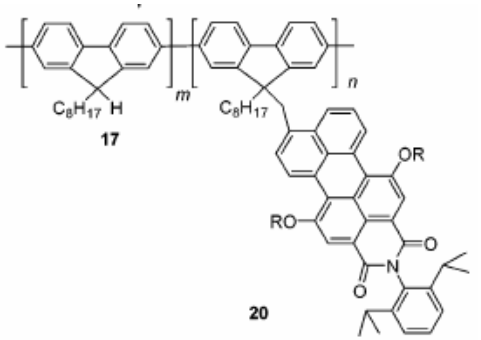
PF

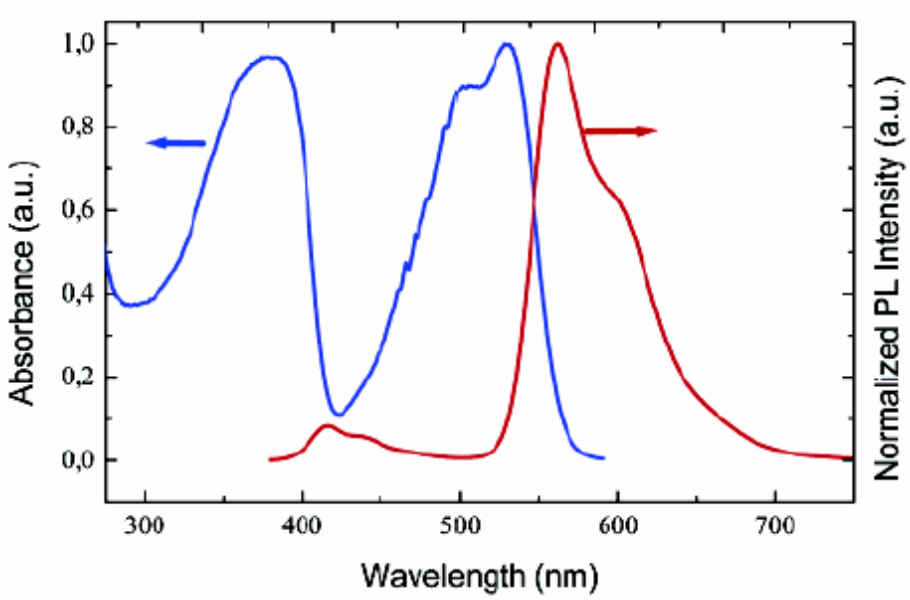
UV-vis Spectroscopy of polyfluorene -- another example



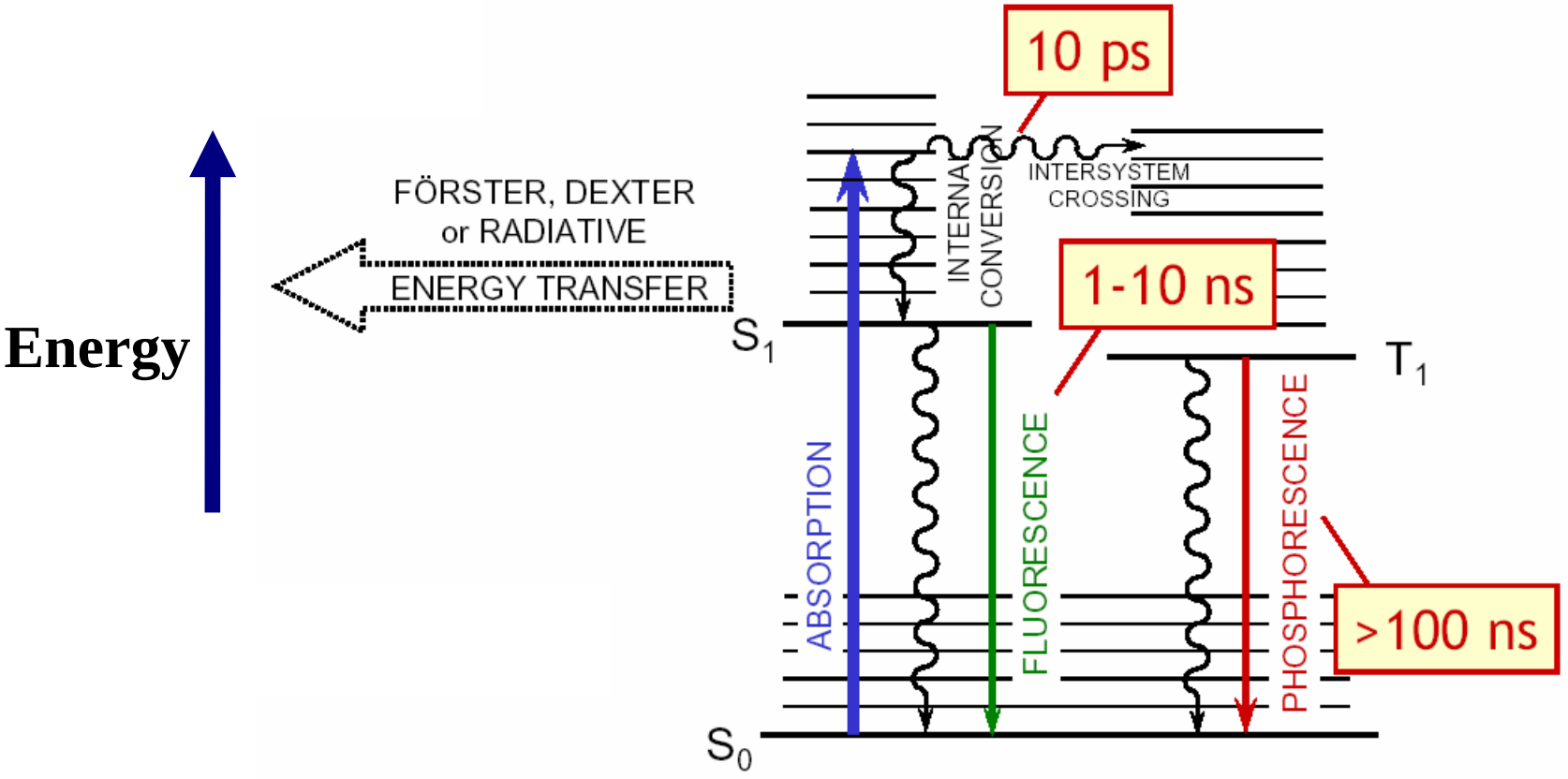
Photoluminescence (PL)





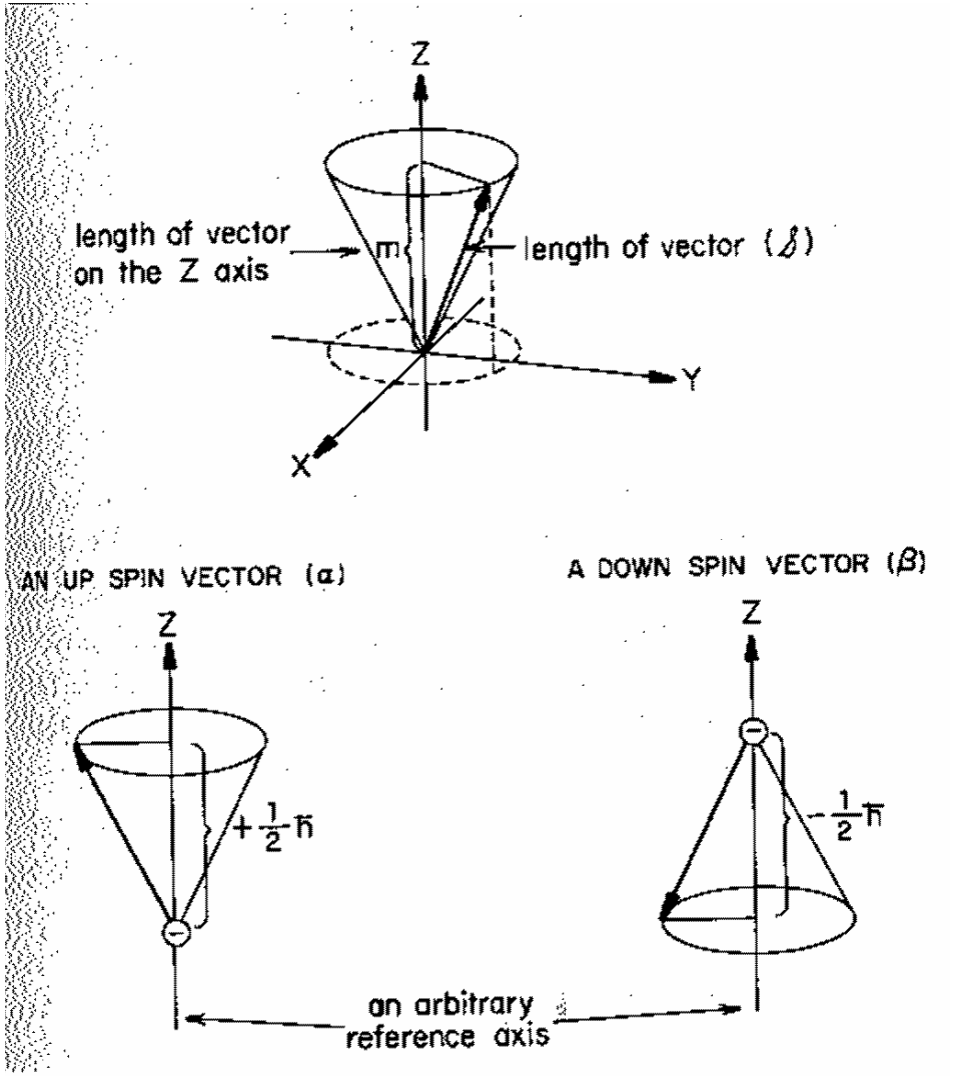


Typical energy levels and energy-transfer process of a molecule

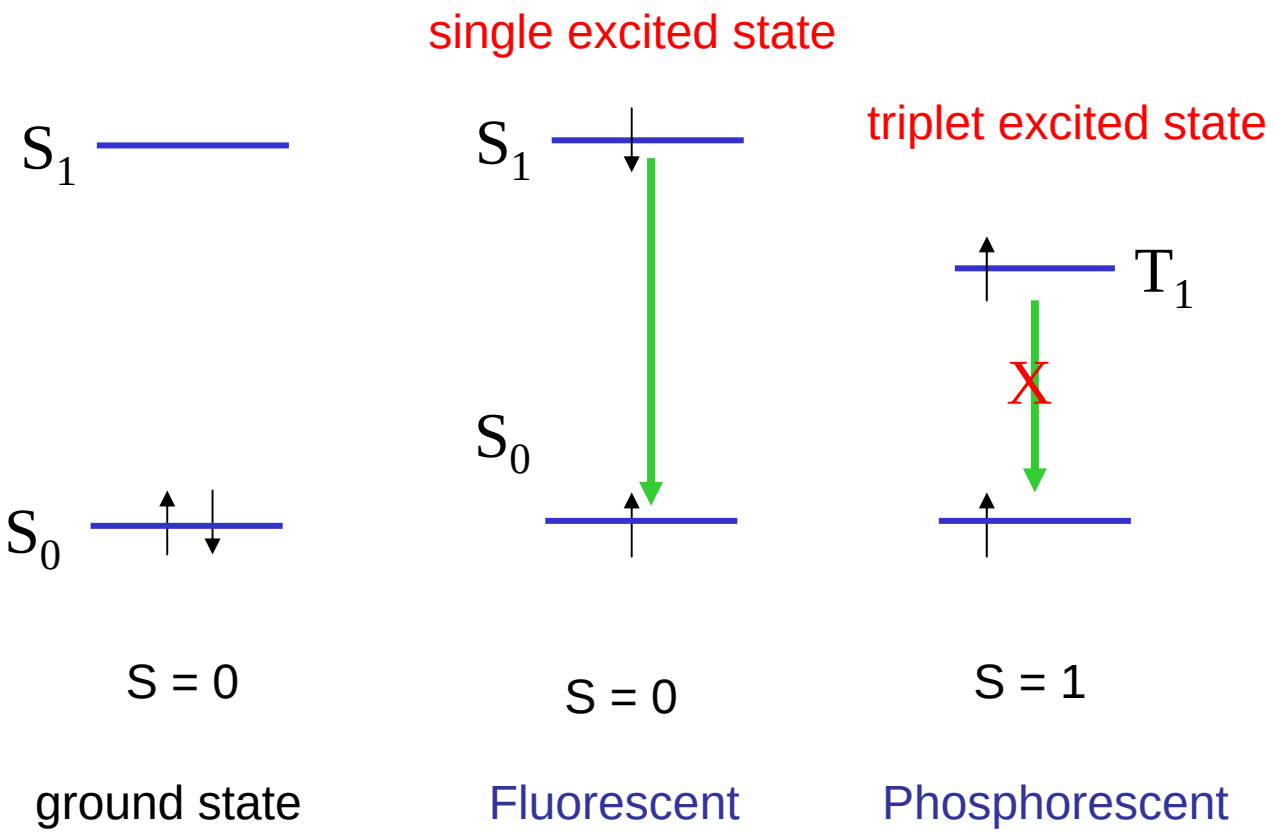


Vector representation of an electron's spin magnet moment

Only two spin states (α, β) are stable



Single and Triplet



Single and triplet states

“up” state
α

“down” state
β