Nanostructural properties 2009/10

Mini-course on fundamental electronic and optical properties of organic semiconductors (part 1)

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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

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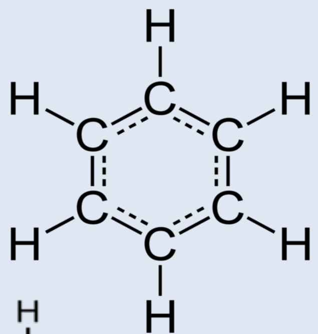
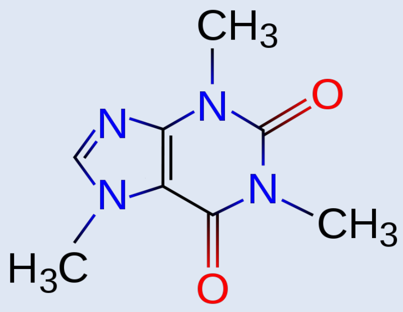
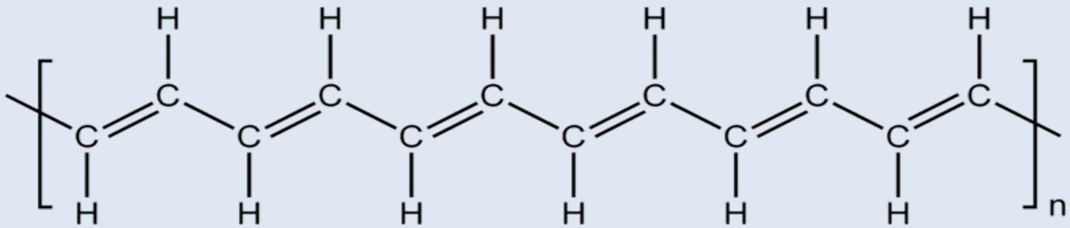
Organic Electronics

- Organic (chemistry):

Organic Chemistry is a discipline within chemistry that involves the scientific study of the structure, properties, composition, reactions, and preparation (by synthesis or by other means) of hydrocarbons and their derivatives. These compounds may contain any number of other elements, including hydrogen, nitrogen, oxygen, the halogens as well as phosphorus, silicon and sulphur [Wikipedia]







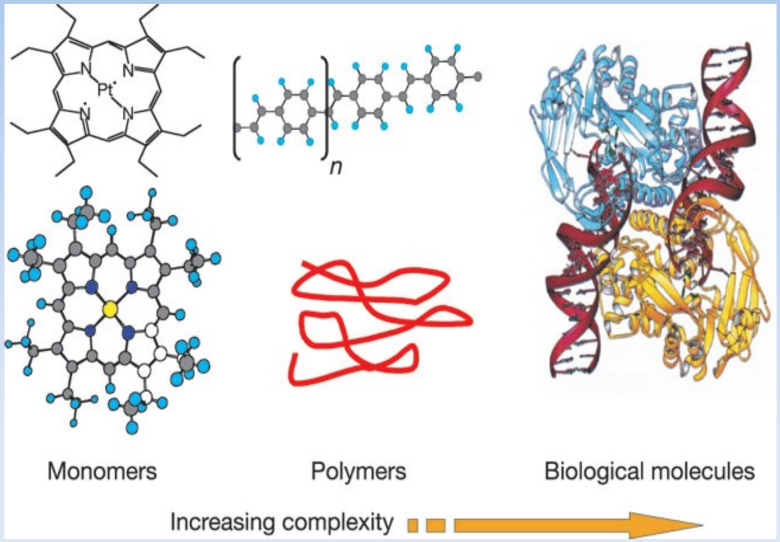
Organic Electronics

- Electronics

Electronics is that branch of science and technology which makes use of the controlled motion of electrons through different media and vacuum.[...] Most electronic devices today use semiconductor components to perform electron control. The study of semiconductor devices and related technology is considered a branch of physics, whereas the design and construction of electronic circuits to solve practical problems come under electronics engineering.[Wikipedia]

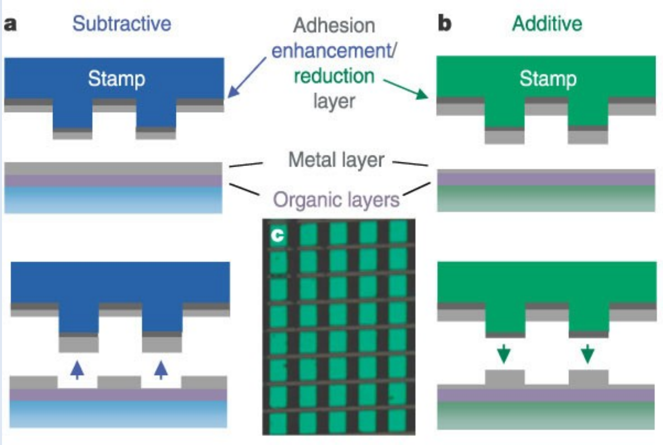
Organic Electronics

S.R.Forrest Nature(2004)



Exploiting the possibilities of organic chemistry

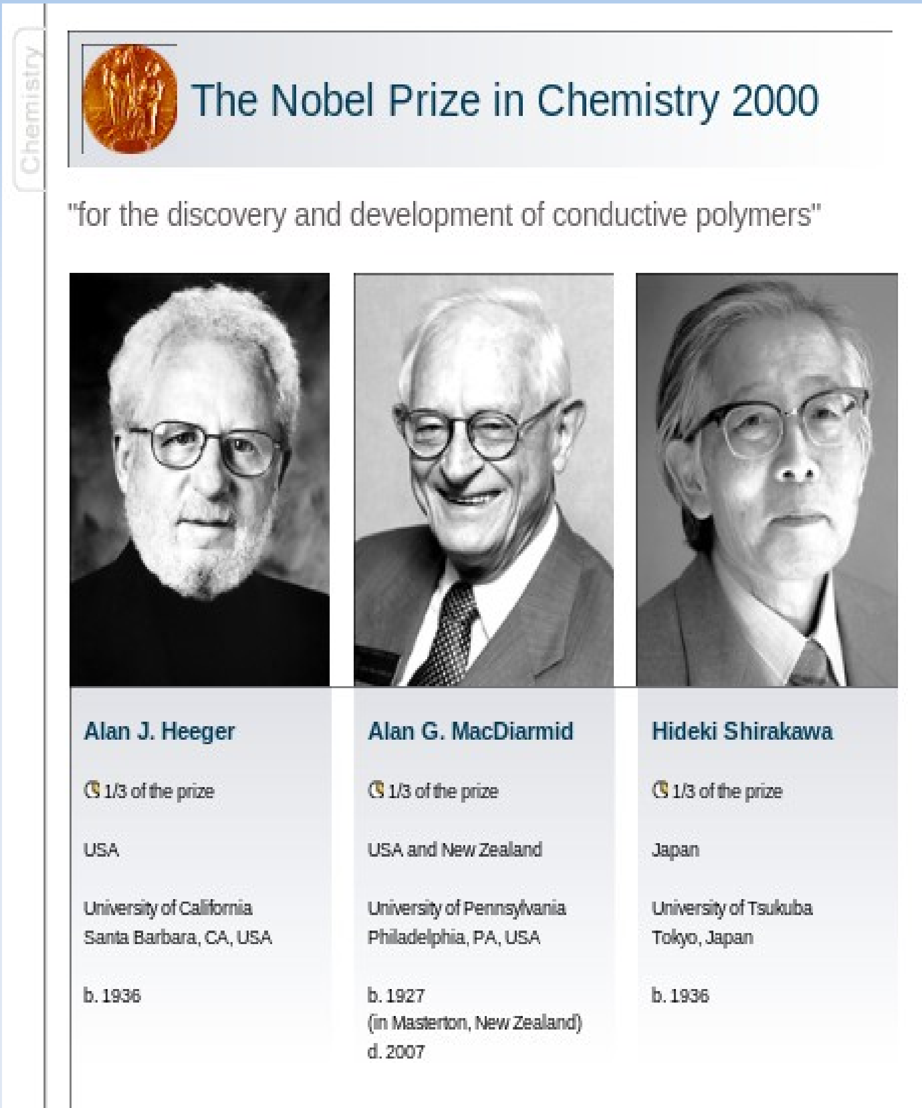
Innovative fabrication methods (solution-based, printing)



Combines good mechanical and electric properties

Plastic Electronics!

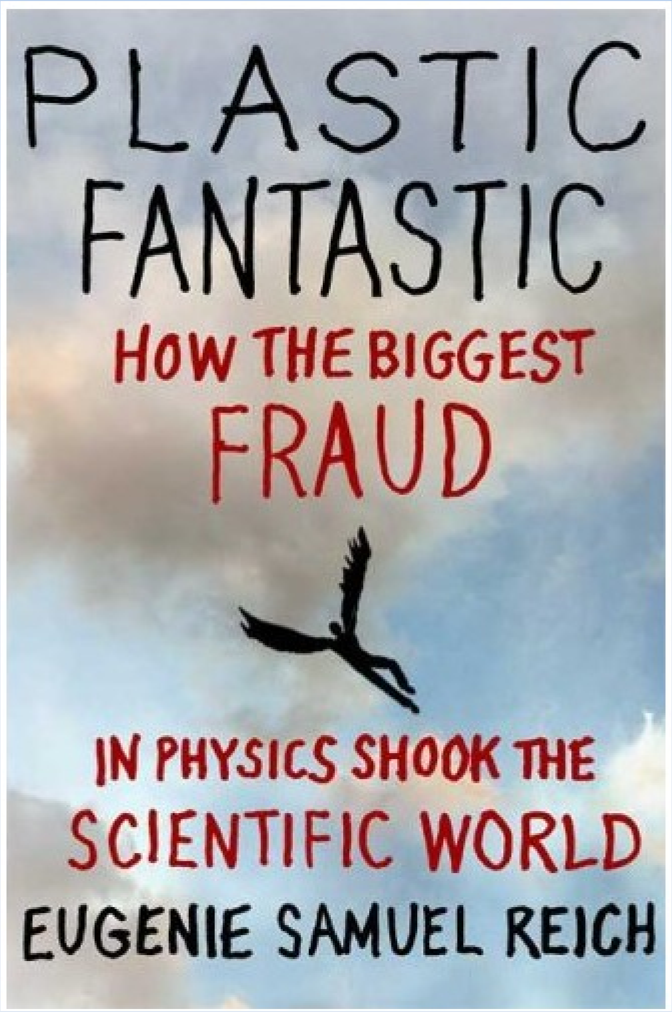
Nobel Prize...



http://nobelprize.org/

Semiconducting polymers

… and scientific fraud!

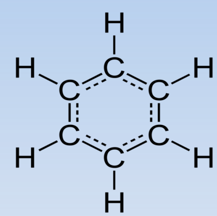


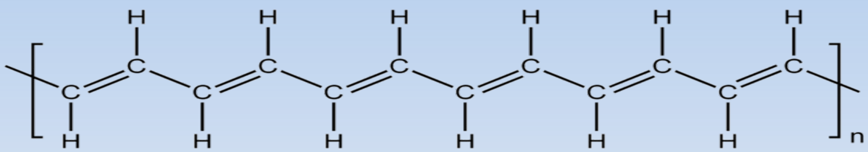
Jan Hendrik Schön and his colleague Zhenan Bao at Bell Labs [www.deutsche-welle.de]

High-temperature superconductivity in organic materials

Key Points Previous Lecture

- Molecular structure





- Controlled motion of electrons
- Semiconductivity
- Solar cells and screens – optoelectronics

- Beware of details...

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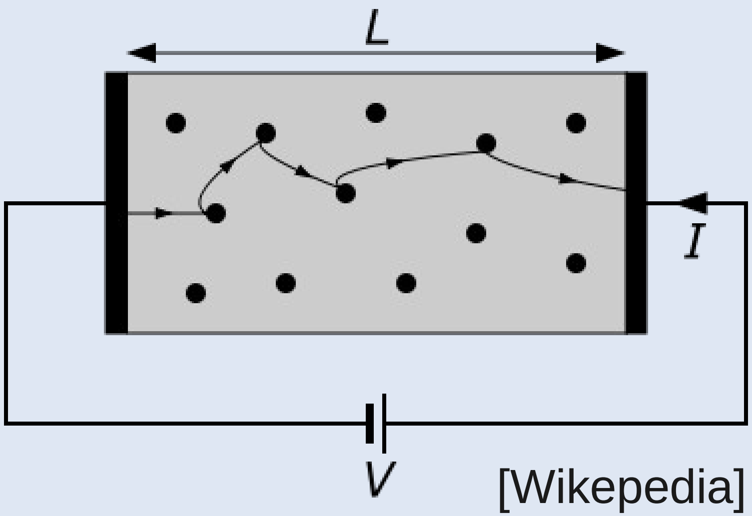
A "Simple" Question

Electronics = controlled motion of electrons

How do electrons move in your device?

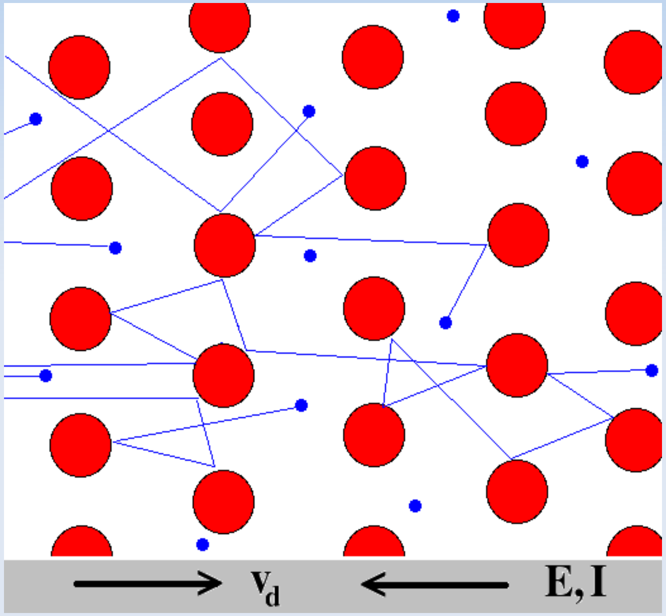


[Wikepedia]

- **Thermal motion**
- **Drift (external field)**
- **Scattering (impurities, lattice vibrations)**
- **Quantum tunnelling**
- **...**

A Simple Answer

Drude theory of conduction (1900)



[Wikepedia]

$$m\dot{v} = qE - \frac{mv}{\tau}$$

Relaxation time

$$\langle \dot{v} \rangle = 0$$

$$\rightarrow \langle v \rangle = \left(\frac{q\tau}{m}\right)E$$

Mobility

$$\rightarrow J = q\langle v \rangle = \left(\frac{q^2\tau}{m}\right)E$$

Conductivity

$$\frac{1}{\tau} = \frac{1}{\tau_{imp}} + \frac{1}{\tau_{ph}} + \cdots$$

All processes contribute

Examples

Mobility [m^2/Vs]

$$\mu = \left(\frac{q\tau}{m}\right)$$

$$q \approx 1.6 \times 10^{-19} C$$

$$\tau \approx 100 \times 10^{-15} s$$

Molecular vibration

$$m \approx 9.1 \times 10^{-31} kg$$

$$\mu \approx 1.7\, m^2/Vs$$

~Metals

Silicon: 0.14 (electron)

2D electron gas (2DEG): ~300

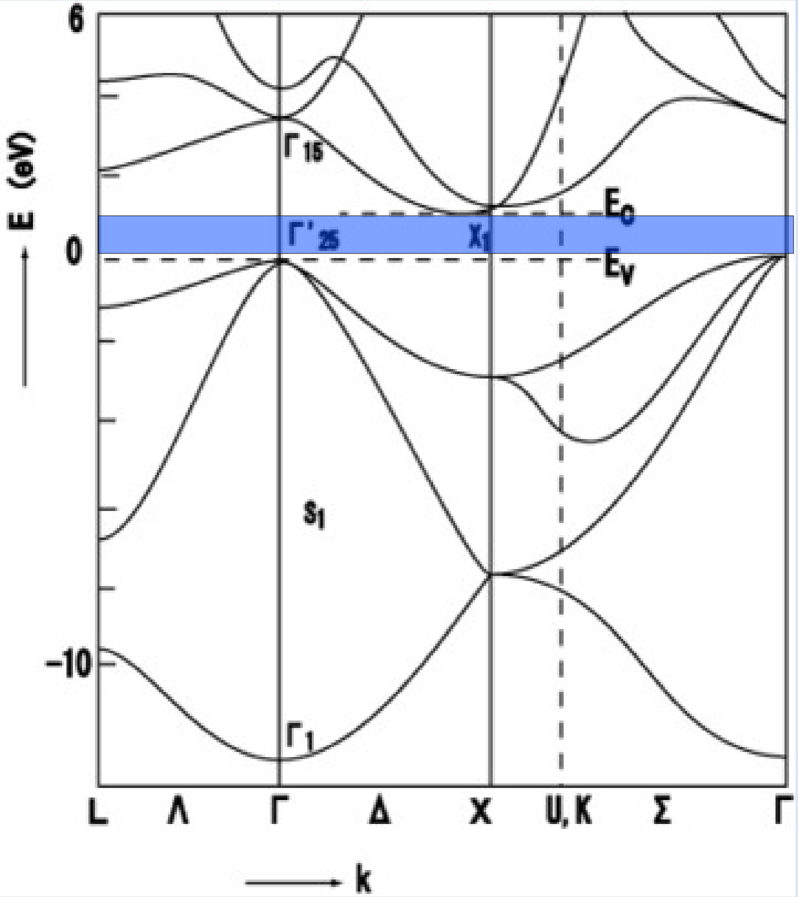
Nanotube: ~ 10.0

Semiconducting polymer: < 0.001

We assumed electrons move freely between two collisions. Is that a good approximation?

Band Theory

Electrons in periodic solids (crystals) interact with the ions (crystal lattice)



Energy bands are like atomic or molecular levels, but depend on a parameter, k

Example: free electrons

$$E_n(k) = \frac{\hbar^2 k^2}{2\text{m}}$$

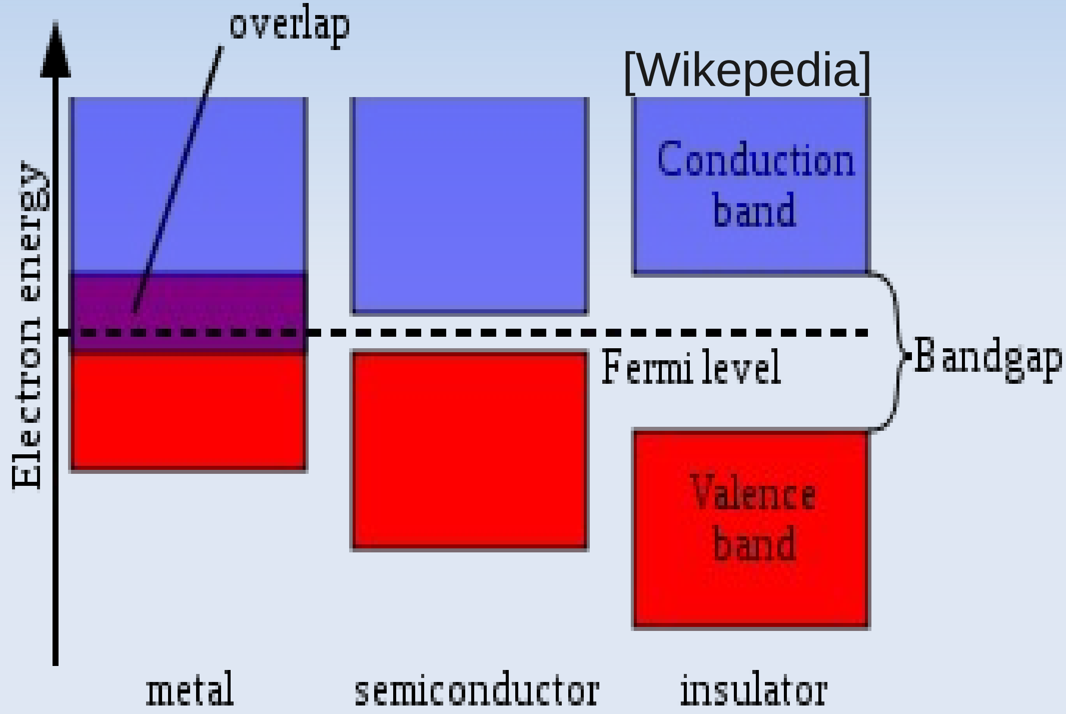
$$\rightarrow v_n(k) = \frac{1}{\hbar}\frac{\partial E_n}{\partial k} = \frac{\hbar k}{m}$$

$$\rightarrow 1/m_n(k) = \frac{1}{\hbar^2}\frac{\partial^2 E_n}{\partial k^2} = 1/m$$

Si, from electronic structure calculations

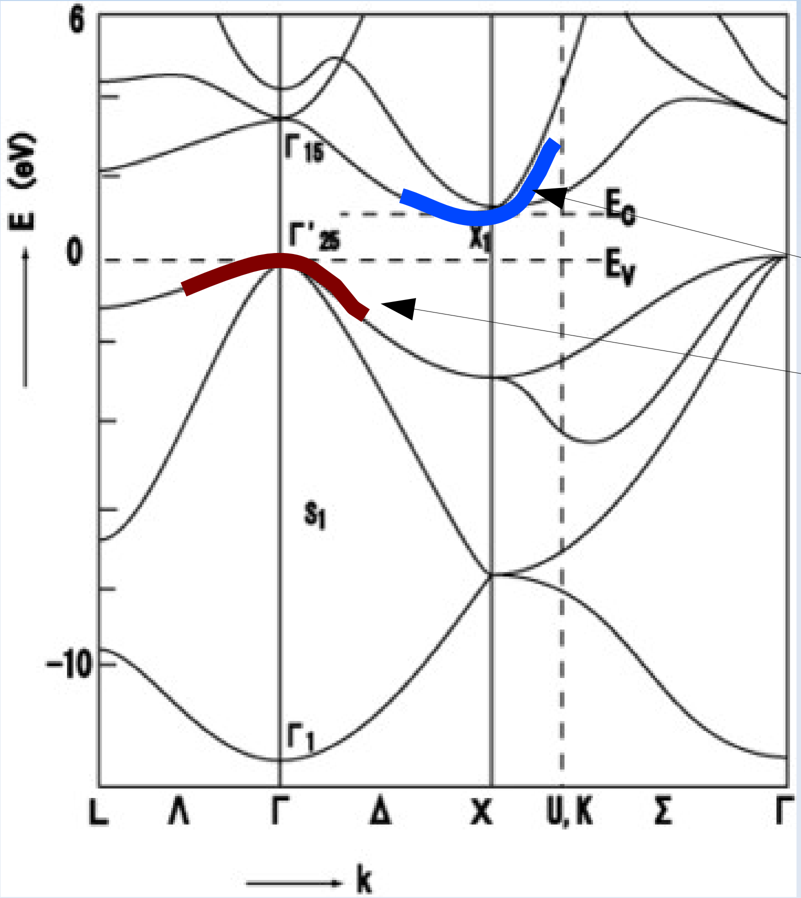
Metal or Insulator?

One can tell from the band structure!



<u>Bandgap</u>: energy needed to create a mobile electron (and a hole)

Electrons and holes



Effective mass: $1/m_{eff} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k^2}$

Electrons: negative, positive mass

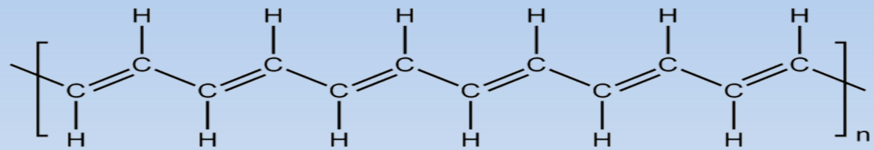
Holes: positive, negative mass

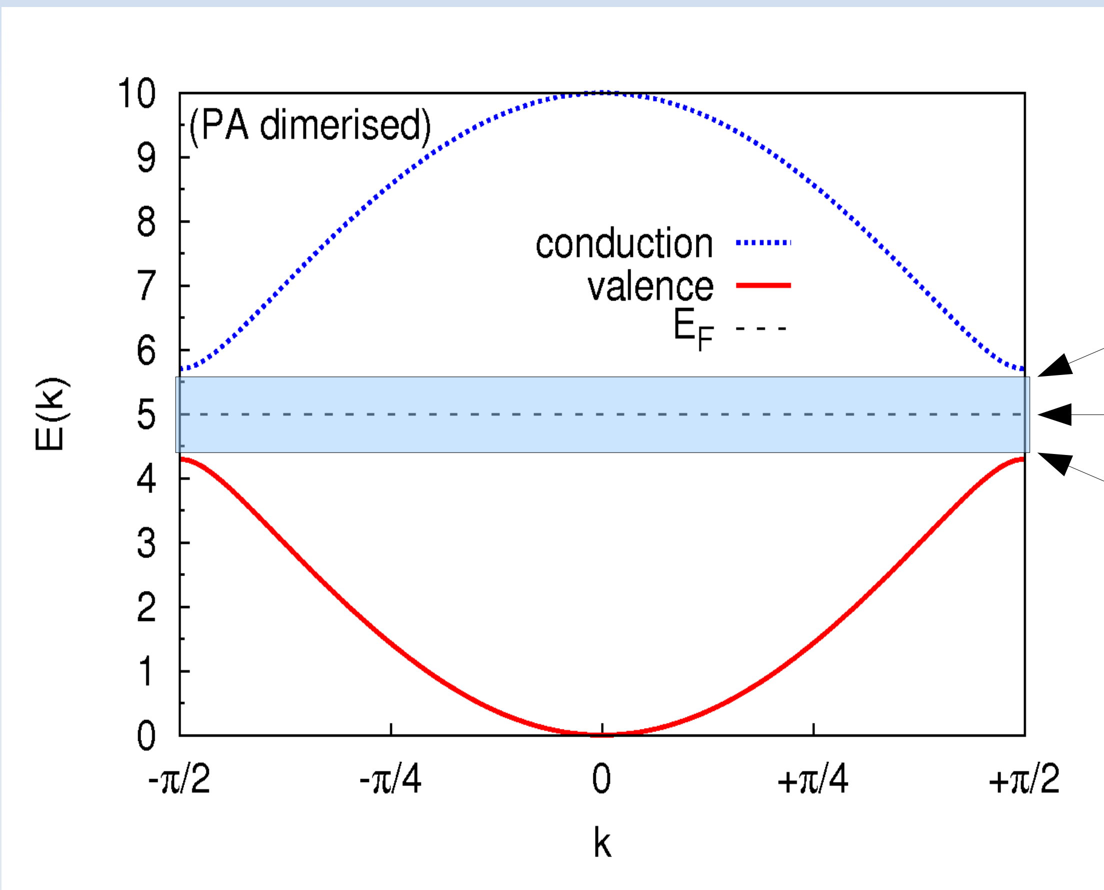
Conductivity:

$$\sigma = \frac{J}{E} = \left(\frac{q^2 \tau_e}{m_{eff,e}} + \frac{q^2 \tau_h}{m_{eff,h}}\right)$$

Polymers ~ 1D Crystals

Polyacetylene (semiconductor)





Electrons

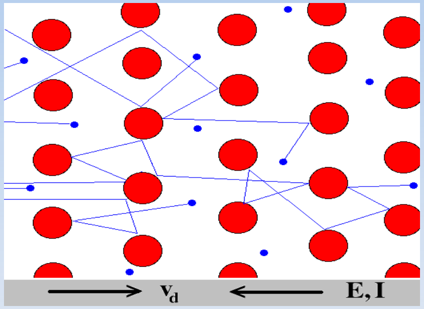
Bandgap

Holes

We shall calculate this band structure!

Key Points Previous Lecture

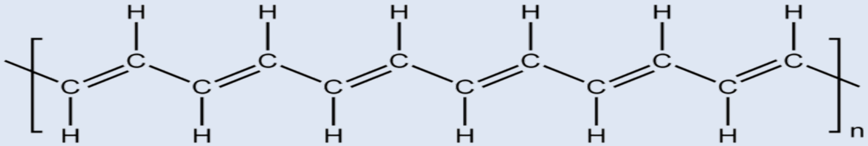
- Original Drude (free electron) model: good for metals



- Band theory: effective mass (electrons&holes) good for semiconductors

$$\sigma = \frac{J}{E} = \left(\frac{q^2 \tau_e}{m_{eff,e}} + \frac{q^2 \tau_h}{m_{eff,h}}\right)$$

- Polymers ~ 1D crystals (first approx. In reality a lot of defects)



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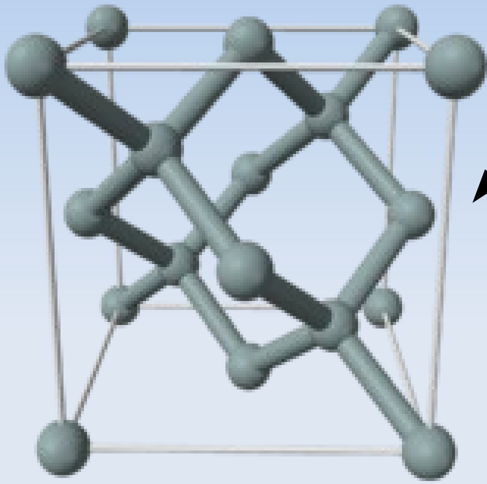
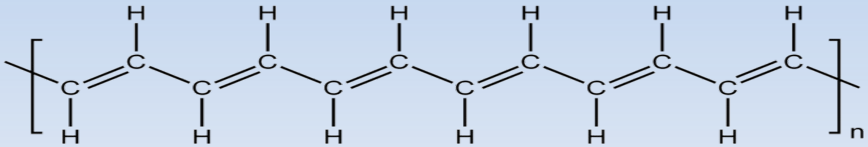
Bonding

Si

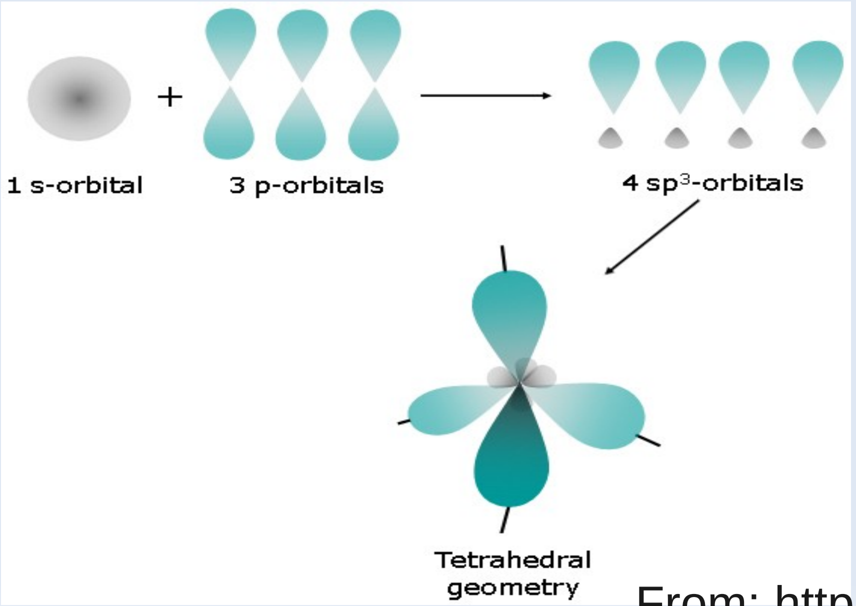


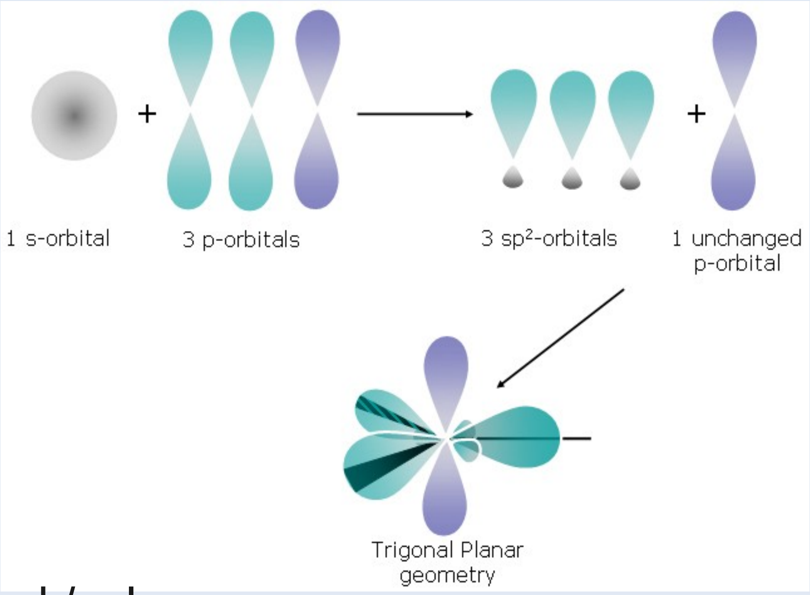
Rigid

PA



Deformable

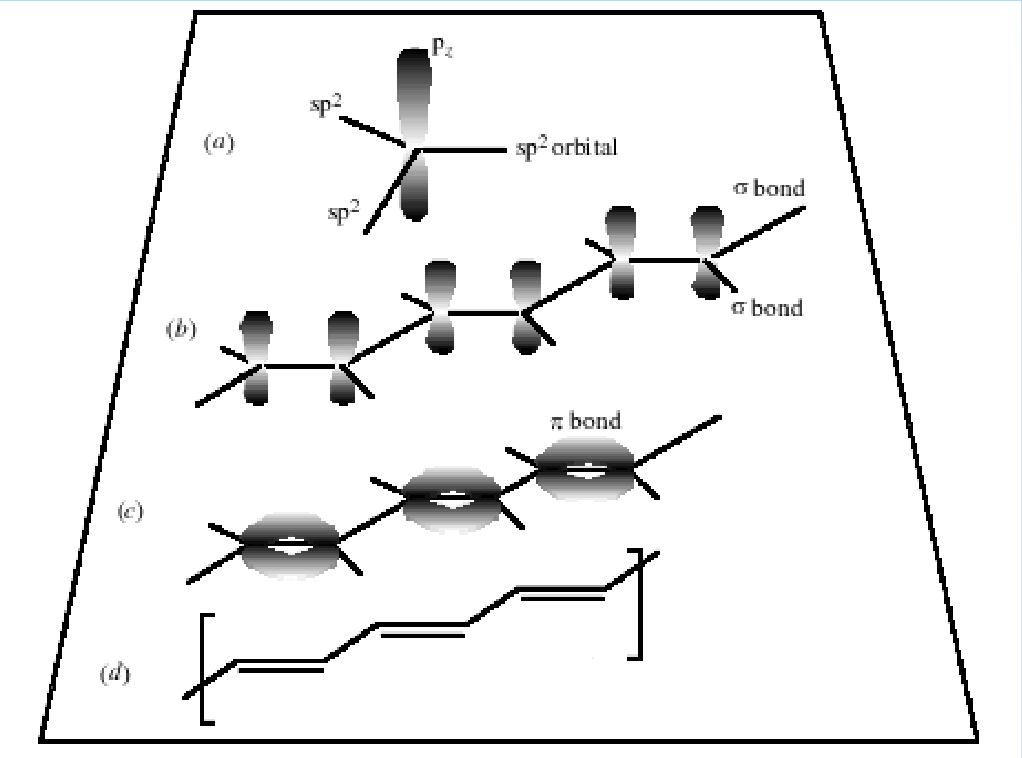




From: http://www.ntu.ac.uk/cels

π-conjugation

Alternation of single and double bonds, <u>Electronic delocalisation</u>

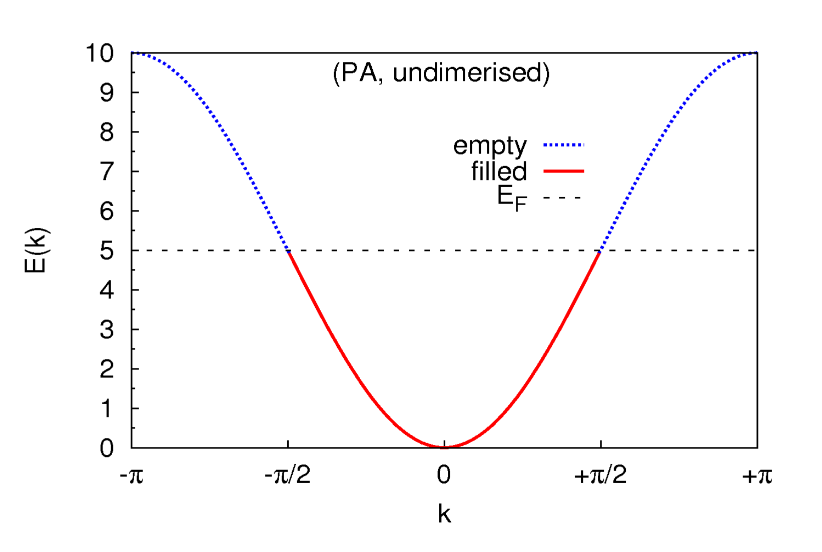


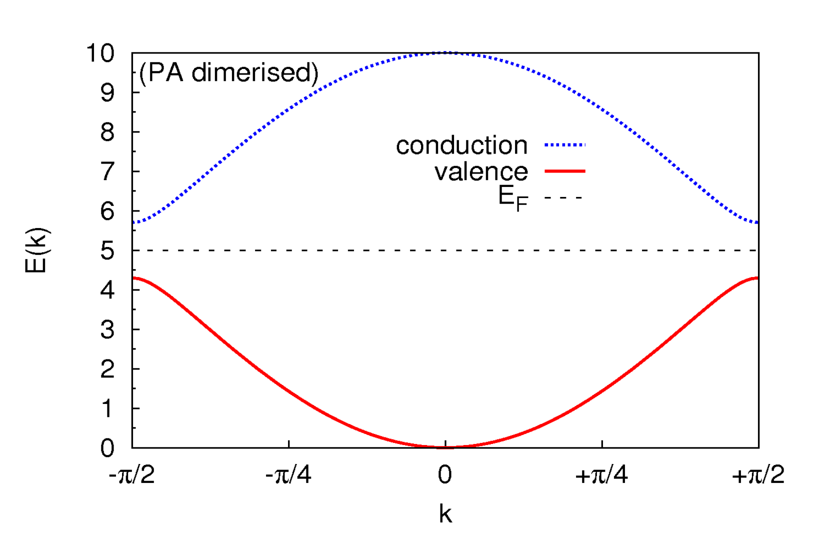
Cacialli, Phil. Trans. R. Soc. Lond. A (2000)

N.B. In reality a lot of defects, <u>finite conjugation length</u>

PA Band Structure (see Notes)

Metal or Semiconductor?
It depends on the <u>structure</u>!





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