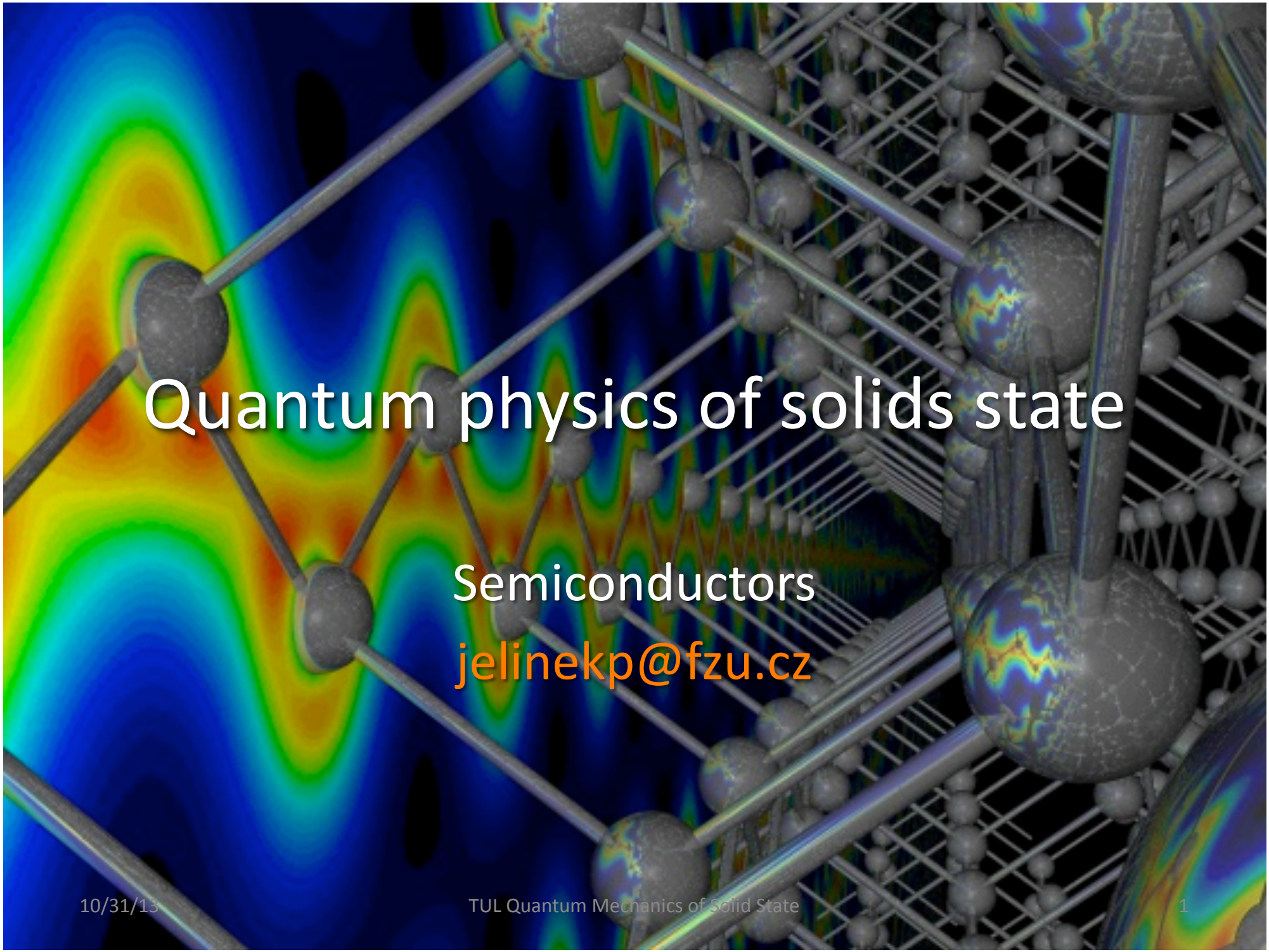


Quantum physics of solids state

Semiconductors

jelinekp@fzu.cz

Transport properties: Drude model

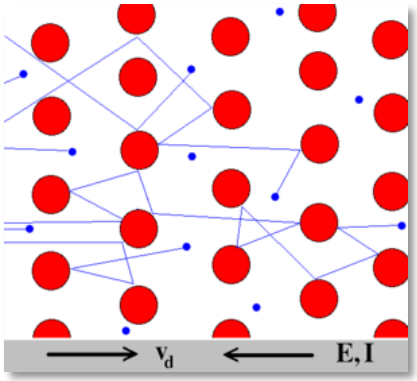
(classical approximation)

Basic assumptions:

- **ideal electron gas** (no interaction with each other)
- e collide with static ions instantaneously
- e reach thermal equilibrium with the lattice through collisions

$$\frac{1}{2}m_e v_t^2 = \frac{3}{2}k_B T$$

- **relaxation time** define time between two e collisions with lattice



eqn. of motion $\frac{d\vec{v}}{dt}m_e = -e\vec{E}$

average drift speed $\vec{v} = \frac{-e\vec{E}\tau}{m_e}$

current density (charge per time) $\vec{j} = -en\vec{v}$

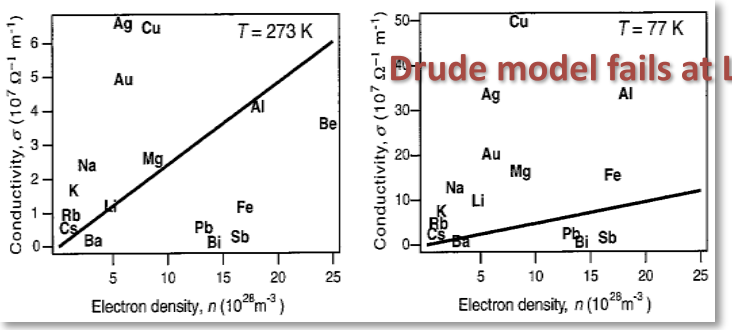
$$\vec{j} = \frac{ne^2\tau}{m_e}\vec{E} = \sigma\vec{E}$$

conductivity

$$\sigma = \frac{ne^2\tau}{m_e}$$

only parameter we need to determine the conductivity is electron density ***n***

Metal	Z_v	n (10^{28} m^{-3})	Measured R_H in units of $-1/ne$
Li	1	4.7	0.8
Na	1	2.7	1.2
K	1	1.3	1.1
Rb	1	1.2	1.0
Cs	1	0.9	0.9
Cu	1	8.5	1.5
Ag	1	5.9	1.3
Be	2	24.7	−0.2
Mg	2	8.6	−0.4
Al	3	18.1	−0.3
Bi	5	14.1	≈40 000

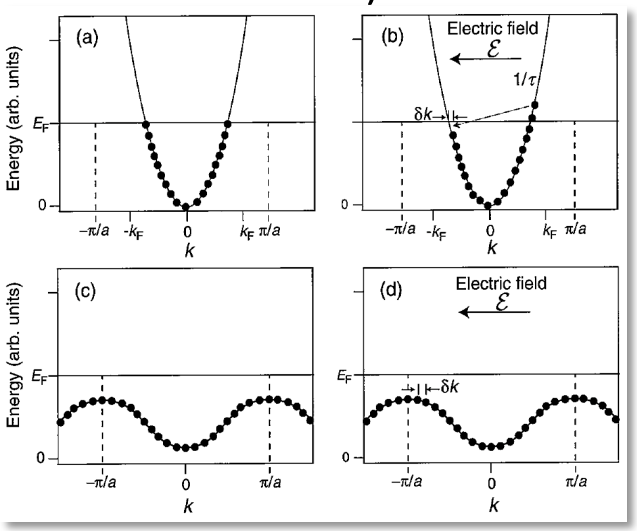


Drude model fails at LT

Transport properties within band structure

(semi-classical approximation)

- the ***Bloch wave*** is ***delocalized over whole crystal*** -> electrons travelling through crystal (stationary solution of S.E.)
- no scattering -> very long (***infinite***) ***mean free path/relaxation time*** (opposite to the Drude model)
- finite relaxation time due to *scattering* with *impurities & lattice vibration* (e-ph interaction)



group velocity $v_g = \frac{d\omega(k)}{dk} = \frac{1}{\hbar}\frac{d\epsilon(k)}{dk}$

acceleration of e- $a = \frac{dv_g}{dt} = -\frac{1}{\hbar^2}\frac{d^2\epsilon(k)}{dk^2}e\vec{E}$

effective mass $m^* = \hbar^2\left(\frac{d^2\epsilon(k)}{dk^2}\right)^{-1}$

m* describes the motion of e- in solids in context of the free electron model

the current depends on the group velocity and density of e- at E_F

conductivity $\sigma = \frac{ne^2\tau_F}{m_F^*}$

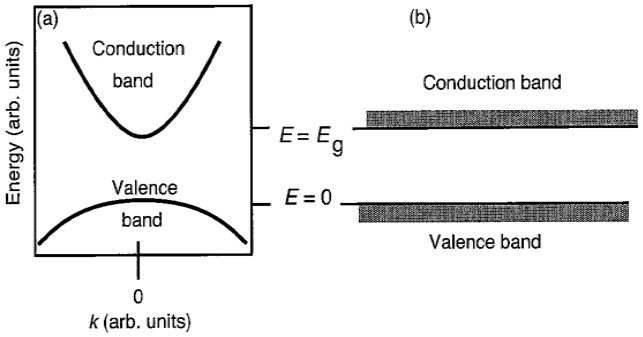
Semiconductor: the band gap

semiconductors characterized by zero DOS at the Fermi level; the band gap

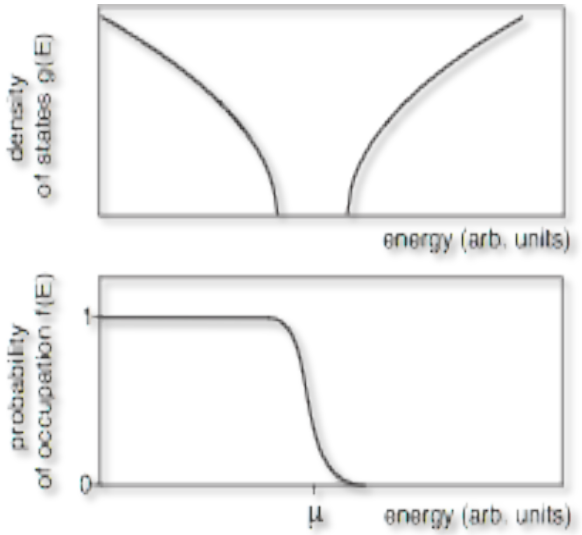
band gap values

	E_g(eV)
InSb	0.18
Ge	0.67
Si	1.11
SiC	2.3
diamond	5.5
MgF_2	11

VB & CB (different m^*)

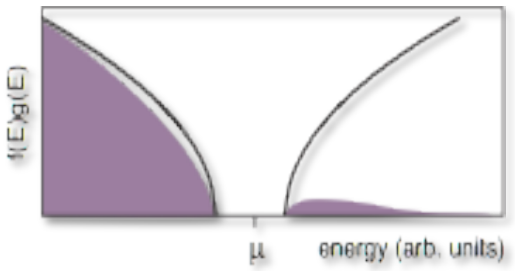


valence band conduction band



- impurities have strong effect on the behavior (doping)

- the Fermi level in middle of the band gap
conservation of number e-

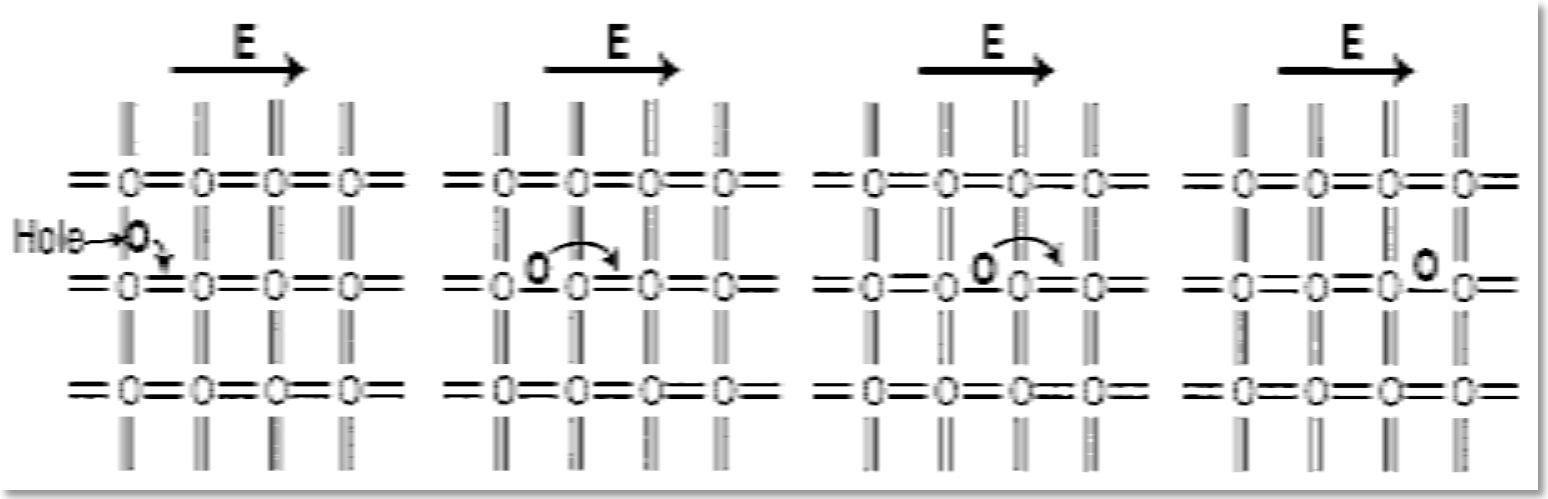


Intrinsic semiconductors

- no impurities
- at finite T presence of e- in CB and hole (missing e-) in VB

hole transport in VB

e- moves in opposite direction to E or equivalently holes moves in direction E



Carrier density vs. temperature

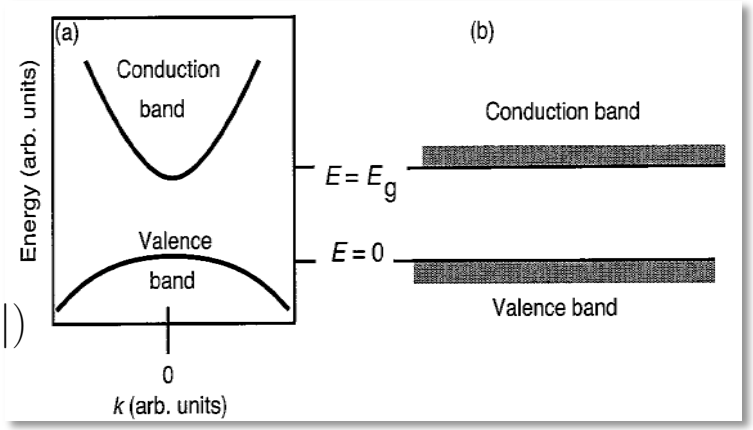
- carrier density determines the transport properties of semiconductors

CB:

$n = \frac{1}{V}\int_{E_c}^{\infty} g_c(E) f(E,T) dE \qquad a = (-e)E/m_e^*$

VB:

$p = \frac{1}{V}\int_{-\infty}^{E_v} g_V(E)(1 - f(E,T)) dE \quad a = (-e)E/(-|m_h^*|)$



the effective mass m* ~ the inverse curvature of a band

where DOS (see L4 p13): $g_c(E)dE = \frac{V}{2\pi^2}\left(\frac{2m_e^*}{\hbar^2}\right)^{\frac{3}{2}}(E - E_g)^{\frac{1}{2}}dE$

$g_V(E)dE = \frac{V}{2\pi^2}\left(\frac{2m_h^*}{\hbar^2}\right)^{\frac{3}{2}}(-E)^{\frac{1}{2}}dE$

electron concentration: $n = 2\left(\frac{2\pi m_e^* k_B T}{h^2}\right)^{\frac{3}{2}} e^{-(E_g-\mu)/k_B T}$

hole concentration: $p = 2\left(\frac{2\pi m_h^* k_B T}{h^2}\right)^{\frac{3}{2}} e^{-\mu/k_B T}$

like Boltzmann distribution with 2 levels, but T hidden in a prefactor

Carrier density vs. temperature II

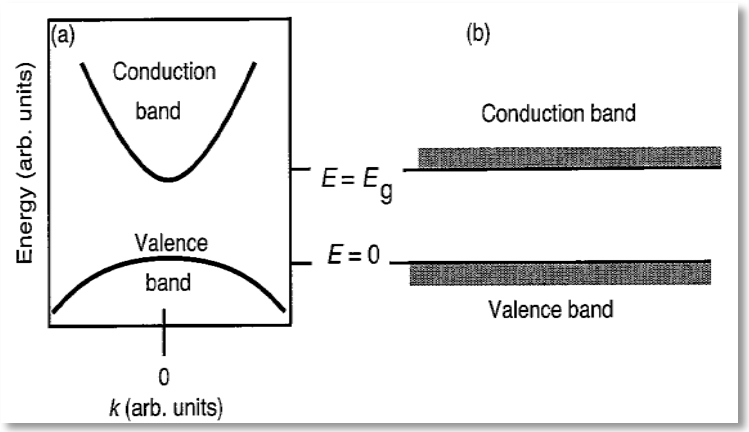
the product n.p independent on the chemical potential

$$np = 4\left(\frac{k_B T}{2\pi\hbar^2}\right)^3 (m_e^* m_h^*)^{3/2} e^{-E_g/k_B T}$$

carrier concentration in intrinsic semiconductor

$$n_i = p_i = 2\left(\frac{k_B T}{2\pi\hbar^2}\right)^{\frac{3}{2}} (m_e^* m_h^*)^{3/4} e^{-E_g/2k_B T}$$

Material	Gap size (eV)	n_i at 150 K (m^{-3})	n_i at 300 K (m^{-3})
Si	1.11	4.1×10^{6}	1.5×10^{16}
GaAs	1.43	1.8×10^{0}	5×10^{13}



the chemical potential determined from the condition n=p

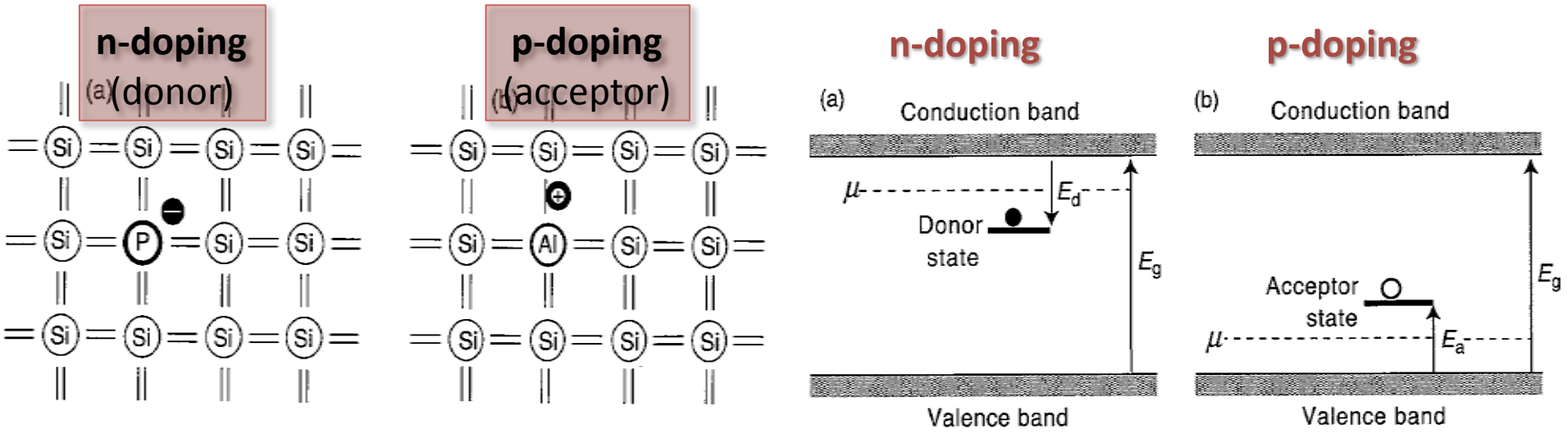
$$\mu = \frac{E_g}{2} + \frac{3}{4} k_B T \ln\left(\frac{m_h^*}{m_e^*}\right)$$

if $m^*_h \sim m^*_e$ than E_F in middle of the gap

Material	m_e^*/m_e	m_h^*/m_e
Ge	0.60	0.28
Si	0.43	0.54
CdSe	0.13	0.45
InSb	0.015	0.39
InAs	0.026	0.41
GaAs	0.065	0.50

Doped semiconductor

doping – adding of **very small amount of alien atoms** (different valence occupancy)
-> formation of **an extra states in the band gap**



free electrons in CB holes in VB

hosting IV-group crystal: sp^3 hybrid orbitals with 4 valence e-

n-doping:

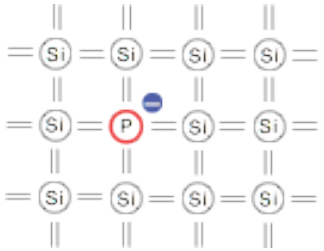
- P, As or Sb with 5 valence e-
- an extra electrons has very small E_b -> easy thermal excitation

p-doping:

- Al, Ga or In with 3 valence e-
- acceptor state can adopt e- from VC by thermal excitation (generating hole in VB)

Fermi level, binding energy

Binding energy: *n*-doping



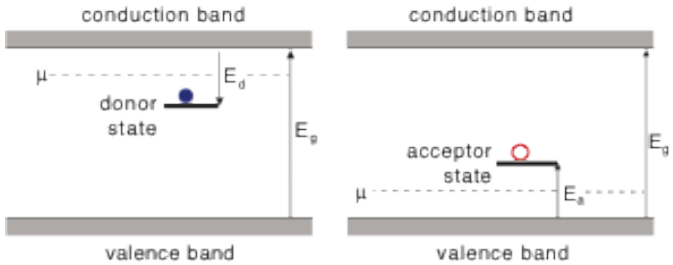
Estimate binding energy with Bohr model: using the modifications

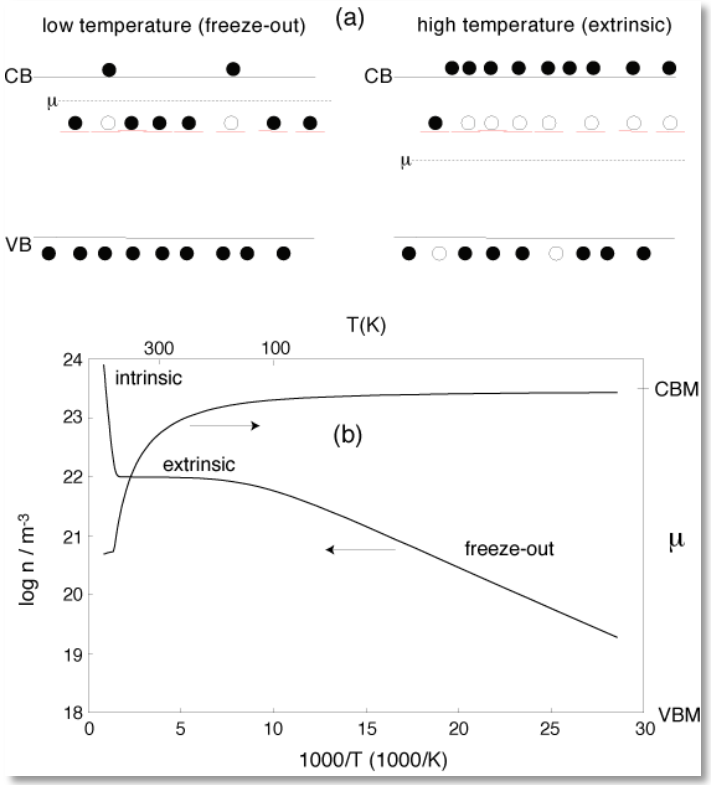
$$E_n = -\frac{m_e e^4}{8\epsilon_o^2 h^2}\frac{1}{n^2}$$

$$m_e \rightarrow m^* \approx 0.43 m_e$$

$$\epsilon_o \rightarrow \epsilon\epsilon_o \approx 11.7\epsilon_o$$

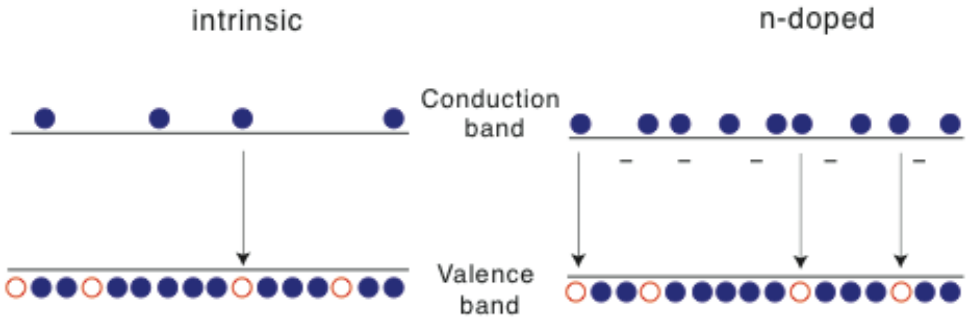
$$E_d = 30\ meV$$





- Only numerical solution possible.
- Basis for calculation is charge neutrality **n=p**.
- At very low temperature, μ must be between donor level and the conduction band minimum (n-doping).
- At very high temperature, μ must be in the middle of the gap because all donors are ionized.

Carrier densities: doping



$$n = 2\left(\frac{2\pi m_e^* k_B T}{h^2}\right)^{\frac{3}{2}} e^{-(E_g-\mu)/k_B T}$$

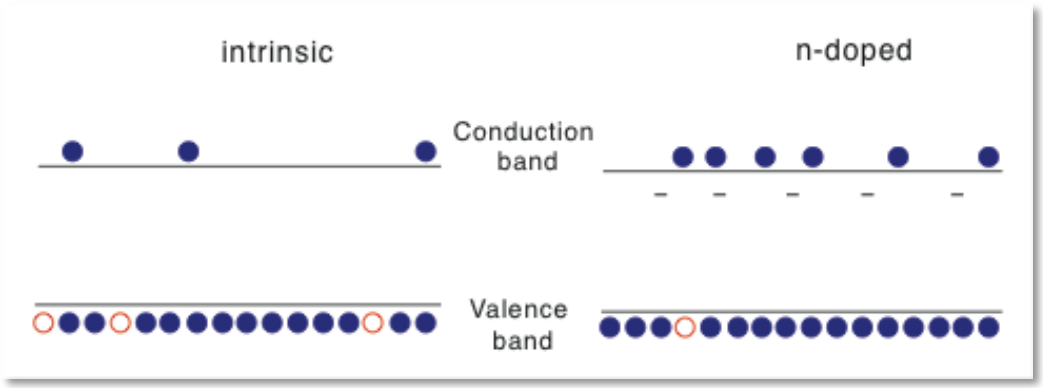
$$p = 2\left(\frac{2\pi m_h^* k_B T}{h^2}\right)^{\frac{3}{2}} e^{-\mu/k_B T}$$

drawback: depend on μ

law of mass action $np = n_i p_i = const$ at a given T

$$np = 4\left(\frac{k_B T}{2\pi\hbar^2}\right)^3 (m_e^* m_h^*)^{3/2} e^{-E_g/k_B T}$$

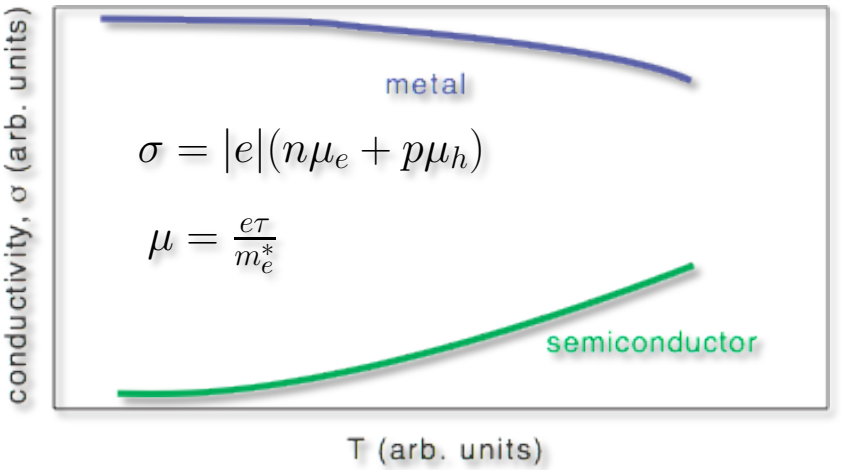
This does not depend on the position of μ.



equal number of electrons and holes

majority: electrons
minority: holes

conductivity



higher T: τ decreases but n,p increases

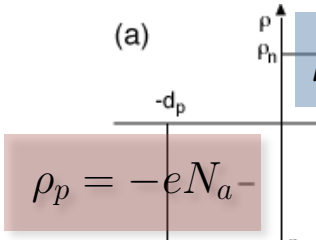
The p-n junction

semiconductor with two region with different doping

an ideal model

Charge density

N_a, N_d ..acceptor(donor) concentration



$$\rho_n = -eN_d$$

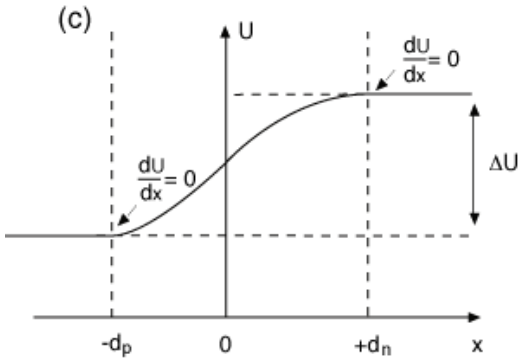
$$\rho_p = -eN_a$$

charge neutrality

$$N_a d_p = N_d d_n$$

Electric field

Electrostatic potential

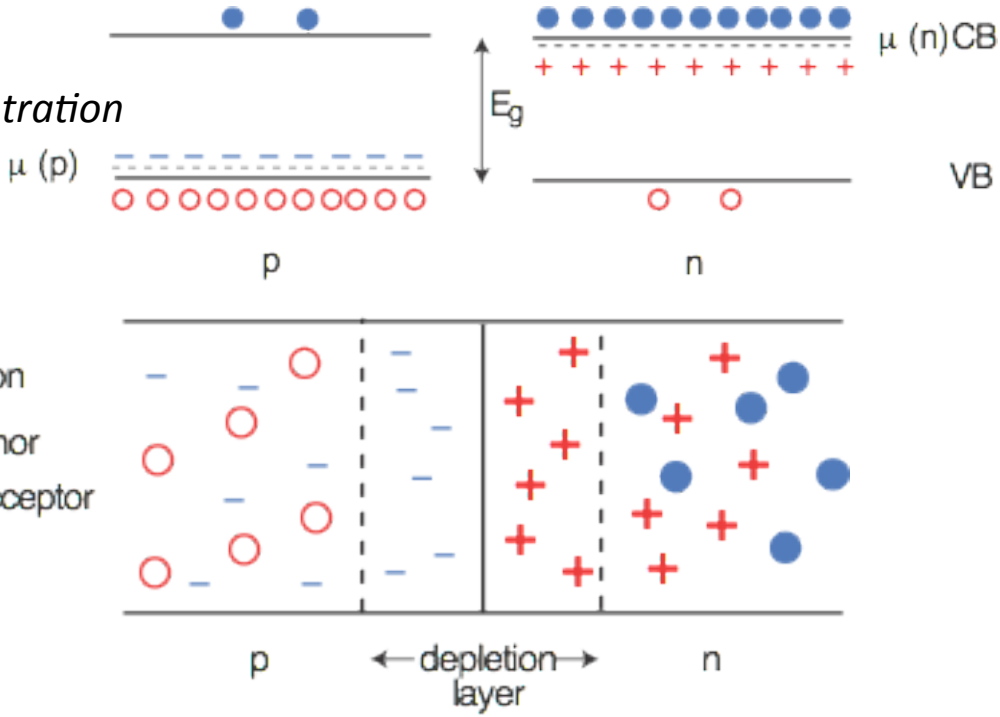


Poisson eqn.

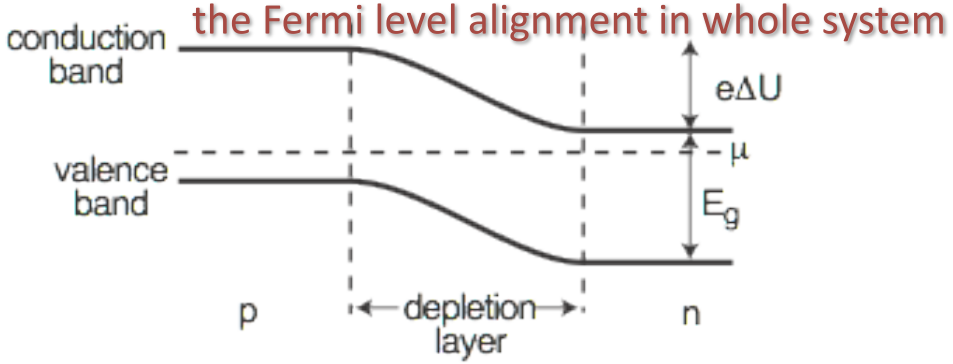
$$\frac{d^2U}{dx^2} = -\frac{\rho}{\epsilon\epsilon_o}$$

$$\frac{dU}{dx}\Big|_{x=-d_p,d_n} = 0$$

$$\Delta U \approx E_g$$



the Fermi level alignment in whole system



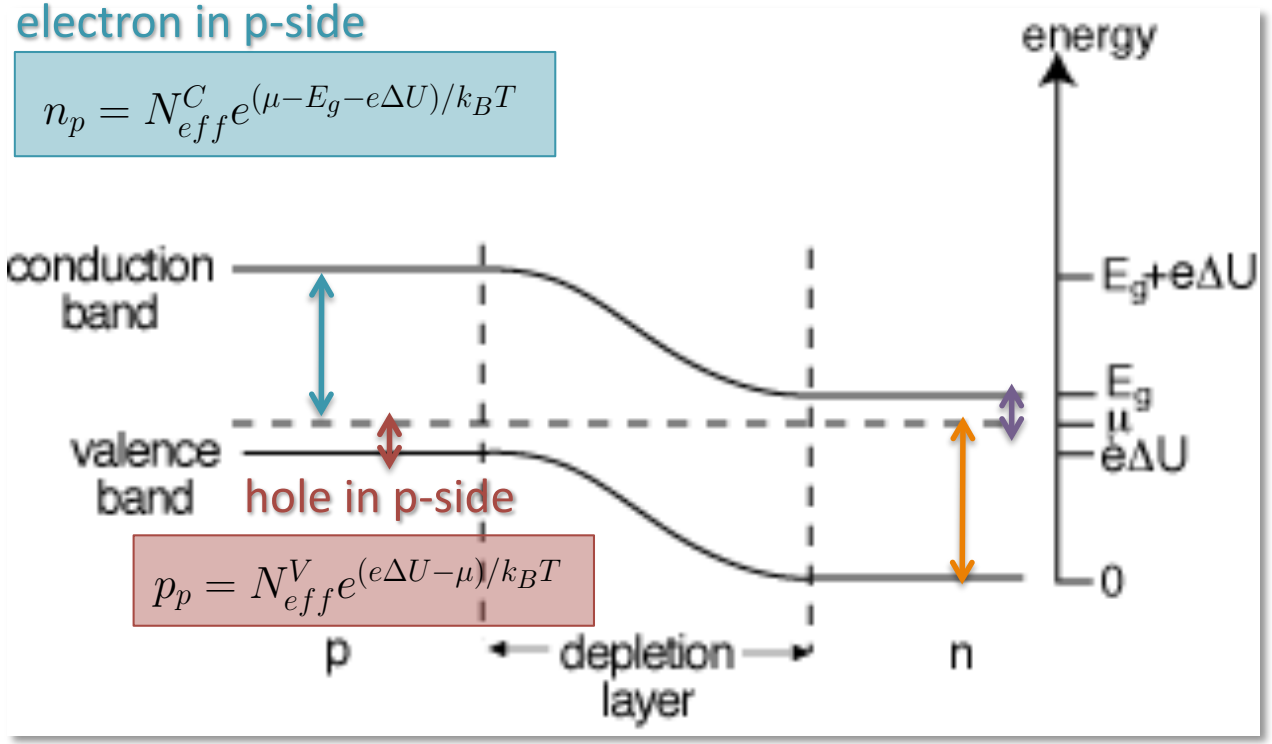
The **depletion layer** length is of the order **0.1 μm to 1μm**

Carrier density: p-n junction

calculate the carrier densities outside the depletion region

electron in p-side

$$n_p = N^C_{eff} e^{(\mu - E_g - e\Delta U)/k_B T}$$



electron in n-side

$$n_n = N^C_{eff} e^{(\mu - E_g)/k_B T}$$

hole in n-side

$$p_n = N^V_{eff} e^{-\mu/k_B T}$$

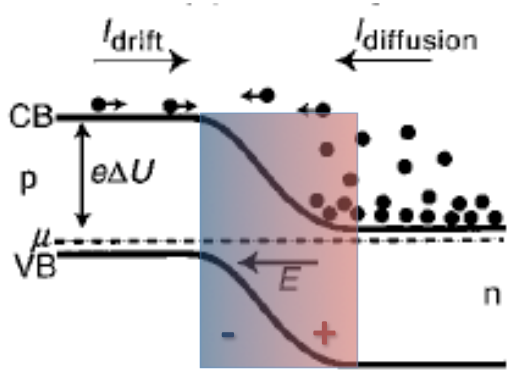
electron/hole statistic

e- $f(E) = \frac{1}{e^{(E-\mu)/k_B T}+1} \approx e^{(\mu - E)/k_B T}$

h+ $1 - f(E) = 1 - \frac{1}{e^{(E-\mu)/k_B T}+1} \approx e^{(E-\mu)/k_B T}$

Transport in p-n junction

there is no zero current across the junction



$$I_{diff} = I_{drift} = I_o$$

$$I_o = Cn_p = Ce^{(\mu - E_g - e\Delta U)/k_B T}$$

drift current: minor e on p-side transferred to n-side by E

diffusion current: mayority e from n-side transferred to p-side due to thermal energy (moves against ele. field in DZ)

forward bias voltage

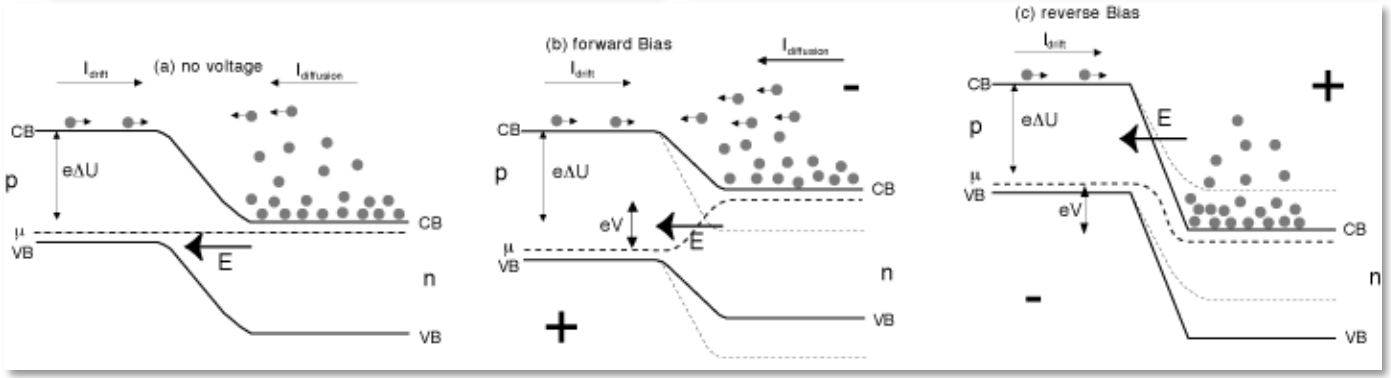
$$I_{diff} = Ce^{((\mu + eV) - E_g - e\Delta U)/k_B T}$$

$$I_o = I_{diff} - I_{drift} = I_o(e^{eV/k_B T} - 1)$$

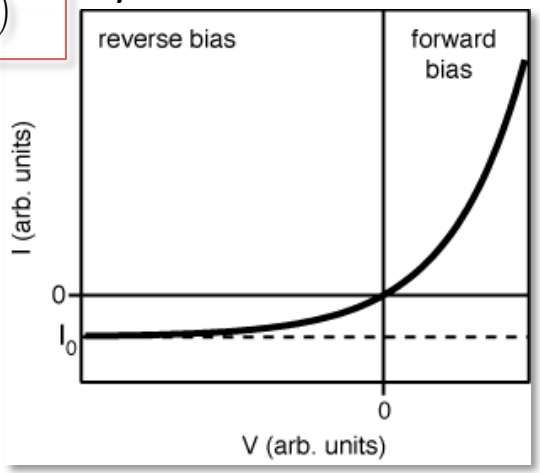
reversed bias voltage

$$I_{diff} = Ce^{((\mu - eV) - E_g - e\Delta U)/k_B T}$$

$$I_o = I_{diff} - I_{drift} = I_o(e^{-eV/k_B T} - 1)$$

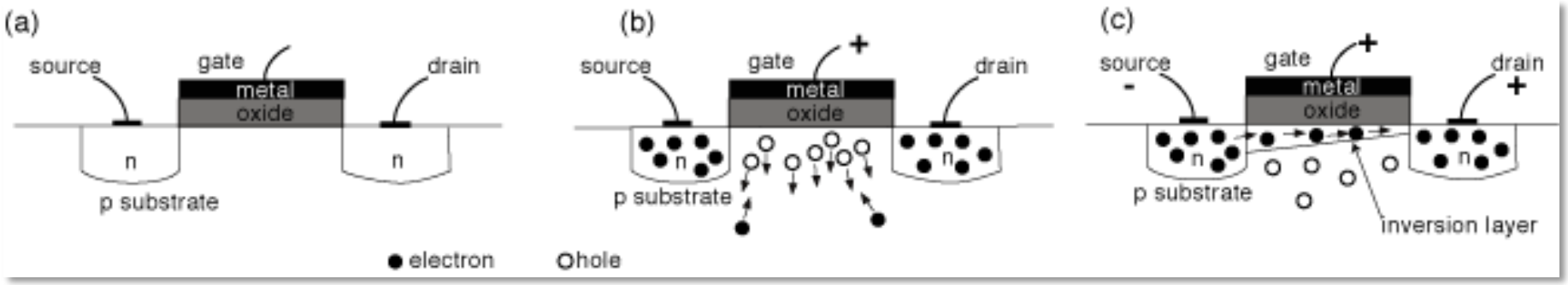


I/V characteristic



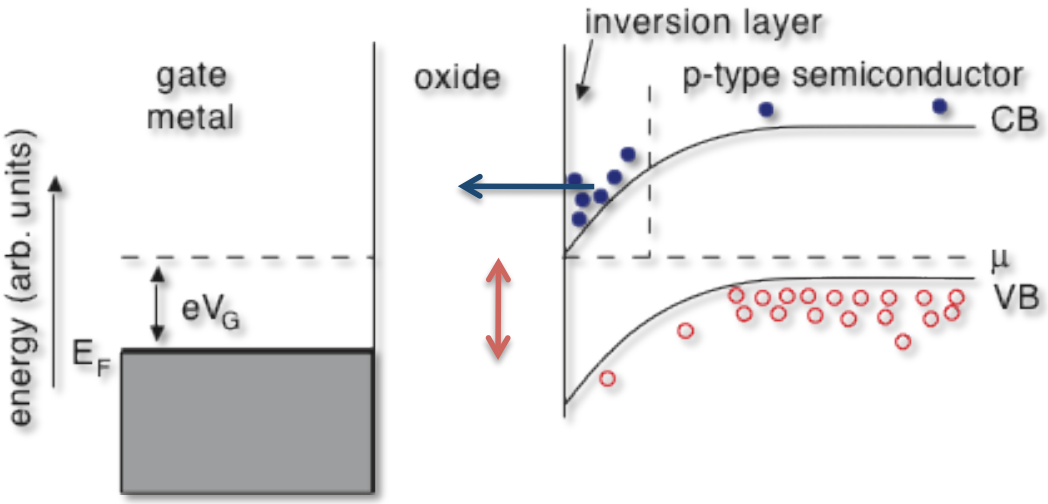
Field Emission Transistors: FET

essential building blocks of microelectronic devices: electrical amplifiers & switches



gate voltage controls the current from the source to the drain

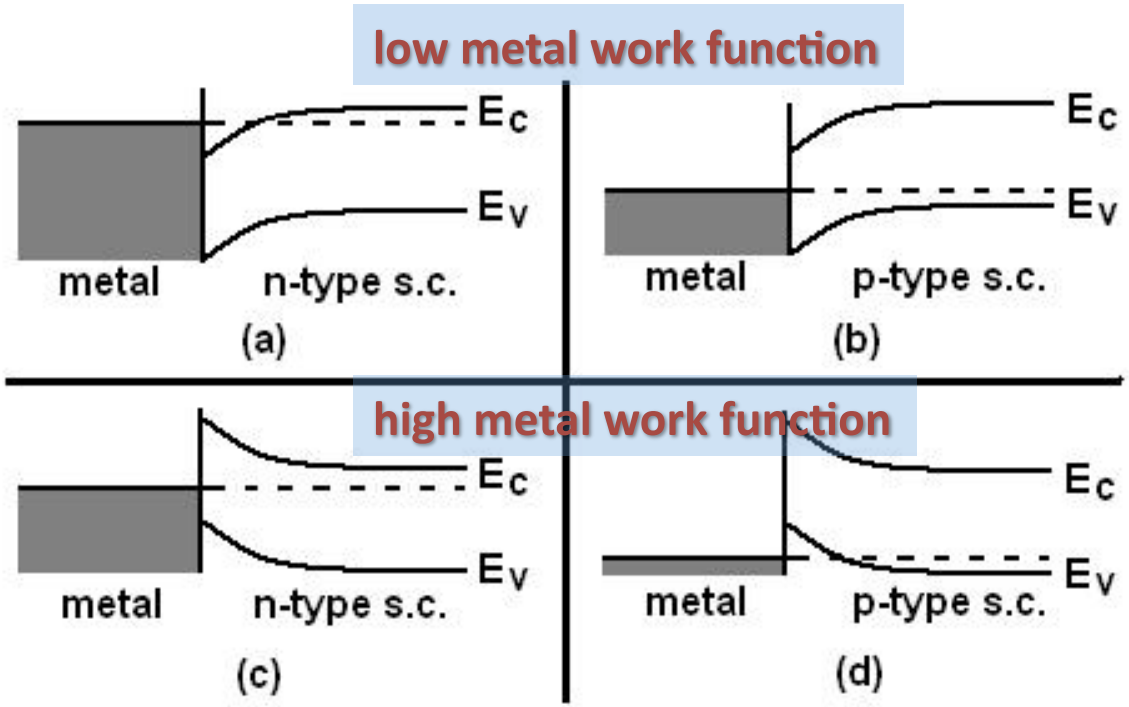
positive voltage applied: the majority h repealed from oxide layers and minority e attracted



sufficiently large gate voltage induces band banding, that the CB gets very close to the Fermi level, than e from CB start to flow.

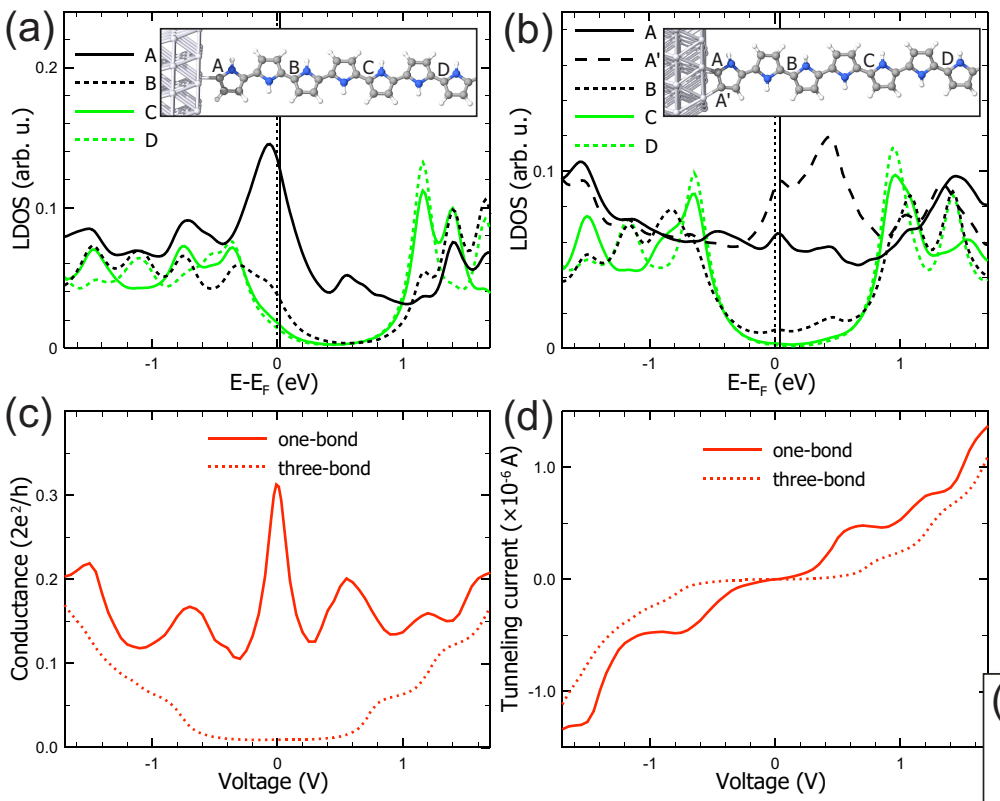
Schottky Barrier

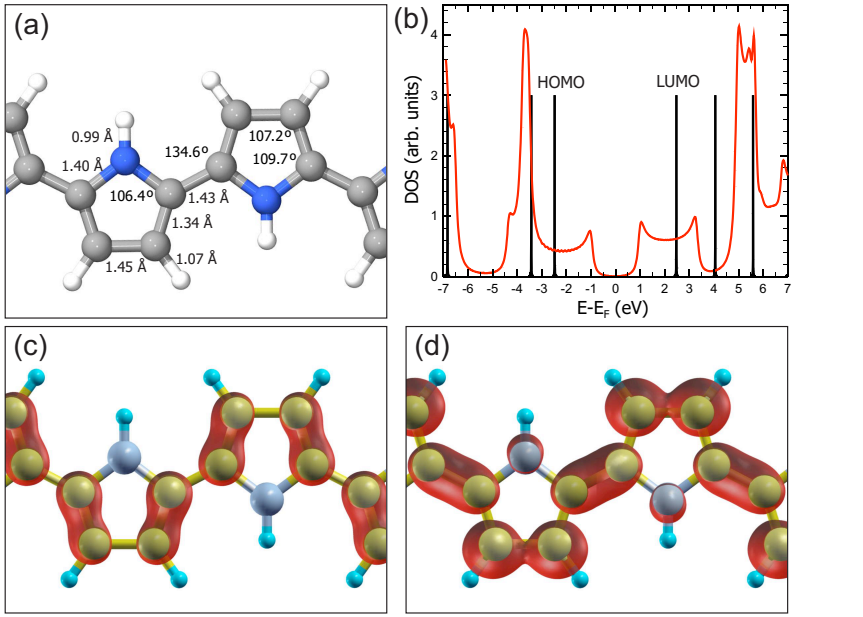
a semiconductor (organic) brought into contact with a metal

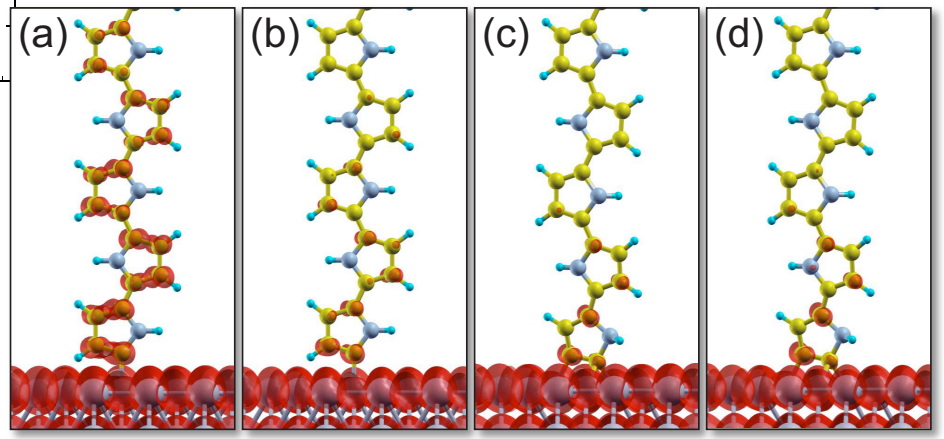


- covalent bonding: induced states in the gap
- charge transfer: formation of interface dipole
- in simple picture: alignment of the vaccum level of both systems

Organic/metal interface



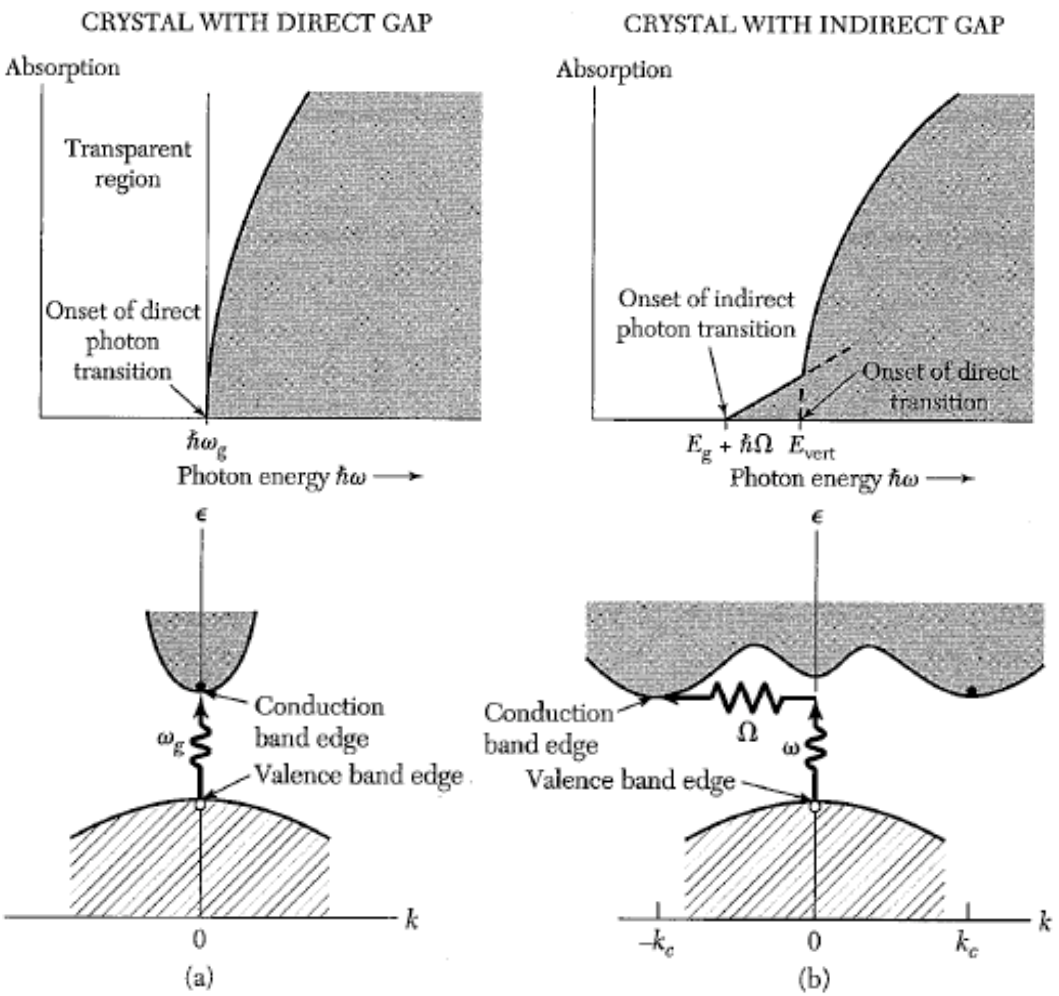




Optical transitions

apart of thermal excitation there is another way to excite an e- from VB to CB

direct absroption process **indirect absroption process**



direct transition

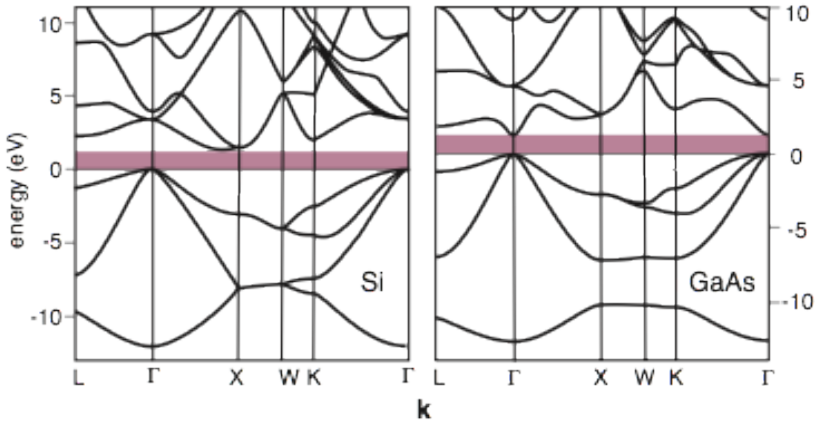
- 2 particles created (e- & h+)

$$E_g = \hbar\omega_g$$

indirect transition

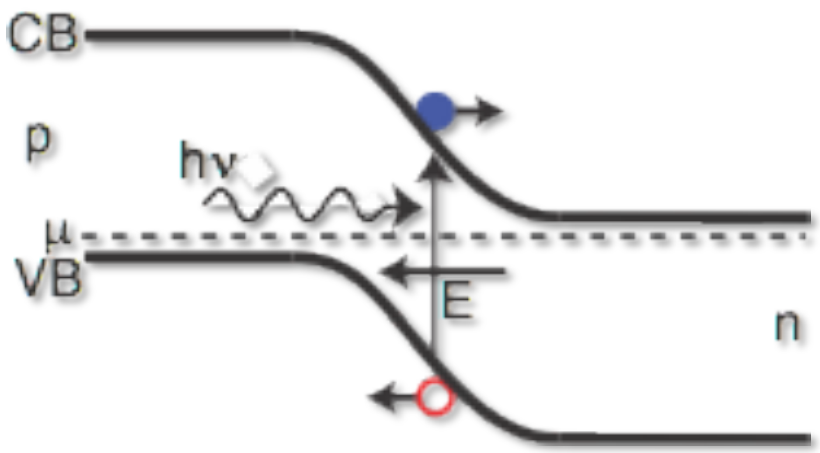
- 3 particles created (e-,h+ & ph)

$$\hbar\omega = E_g + \hbar\Omega$$



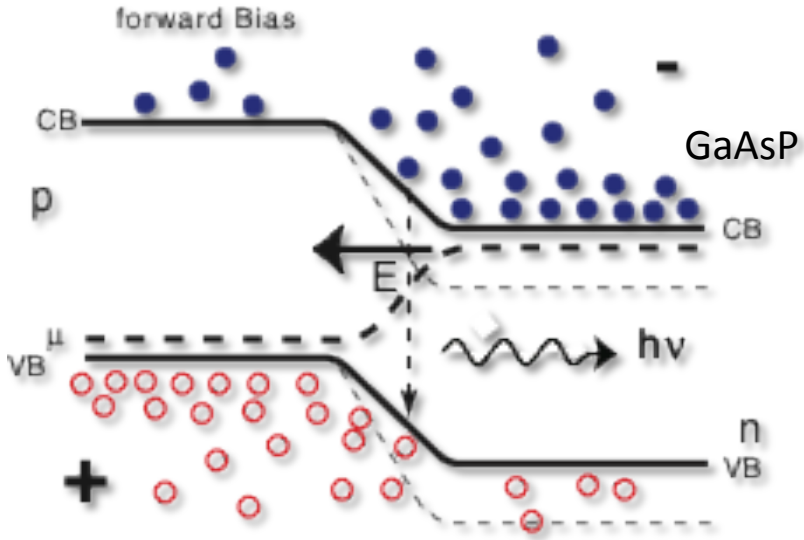
Optoelectronics devices

solar cell



- light induced voltage (current) for reverse-biased diode

LED
(Light Emitting Diodes)



- p-n junction of direct band gap semiconductor operated in forward bias.
- recombination leads to light emission, colour given by band gap.