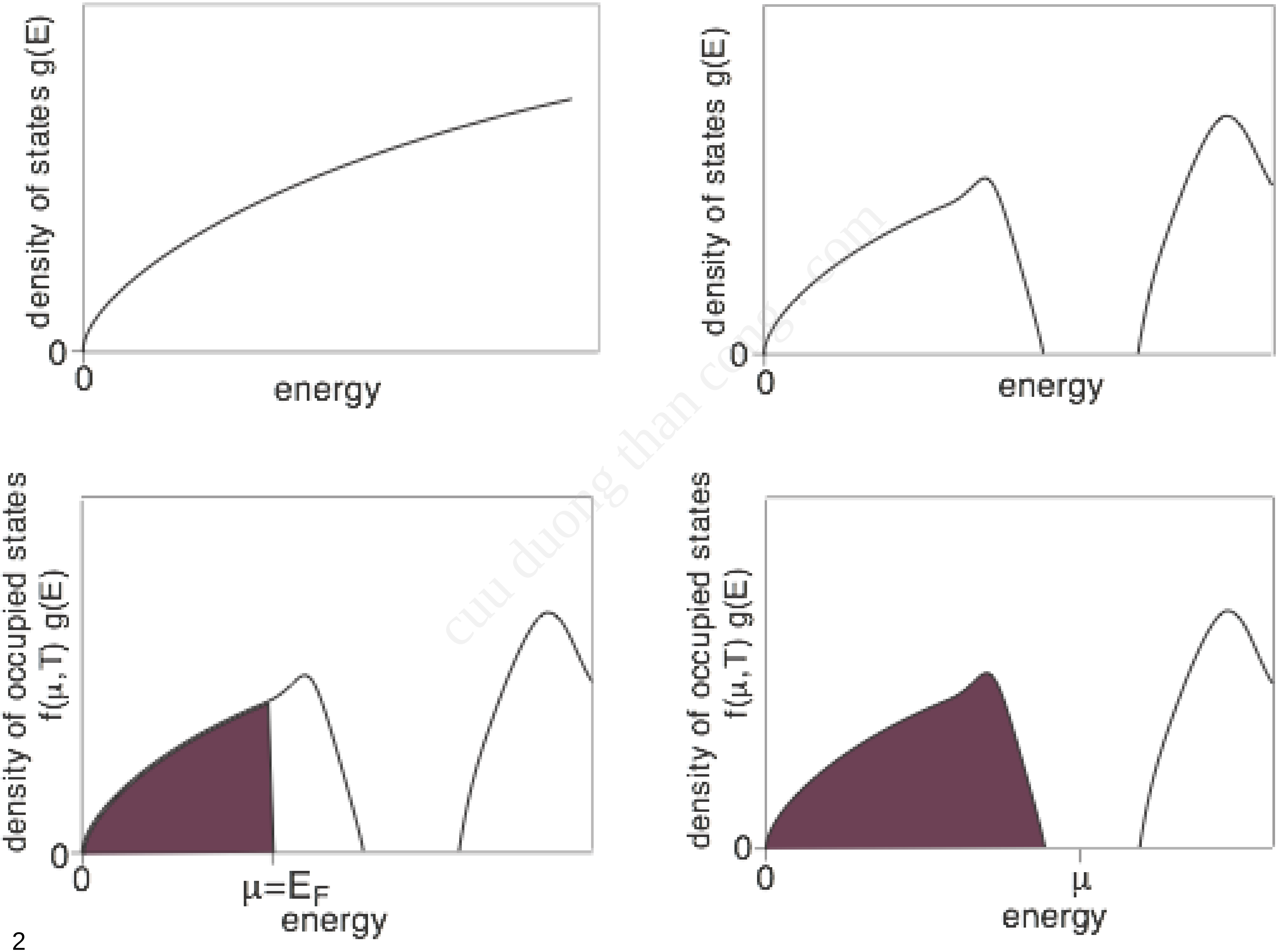
Semiconductors

One shouldn’t work on semiconductors, that is a filthy mess; who knows whether any semiconductors exist.

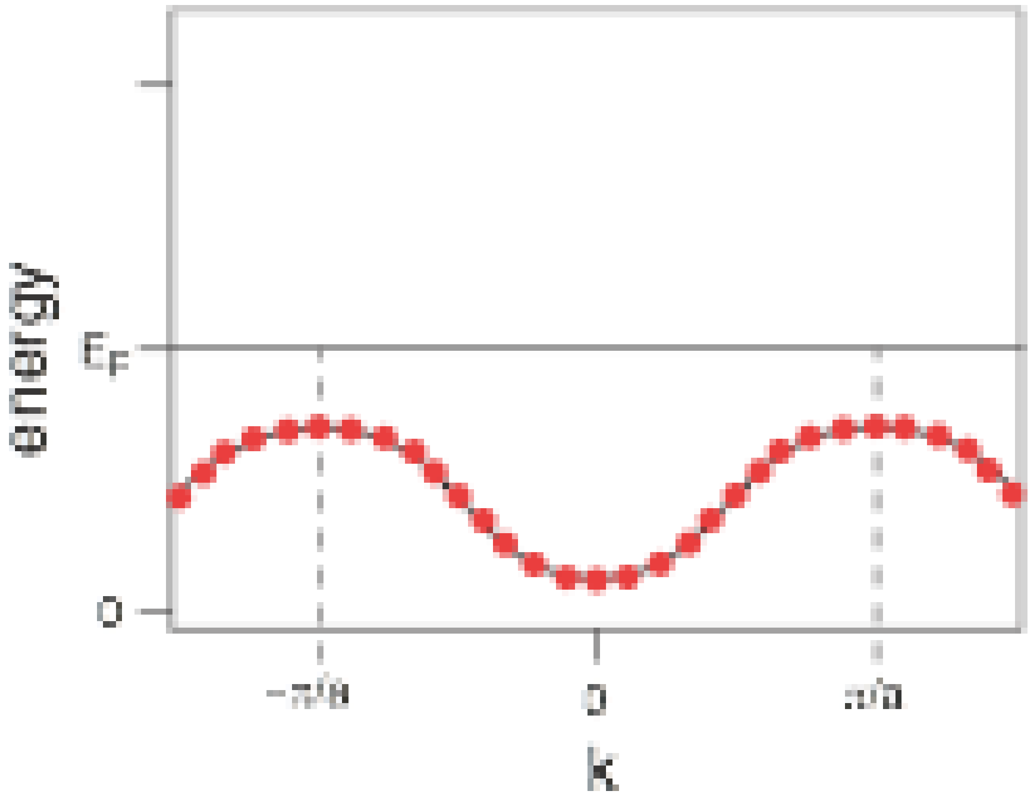
(Über Halbleiter soll man nicht arbeiten, das ist eine Schweinerei; wer weiss, ob es überhaupt Halbleiter gibt.)

Wofgang Pauli, 1931

Metals and insulators / semiconductors



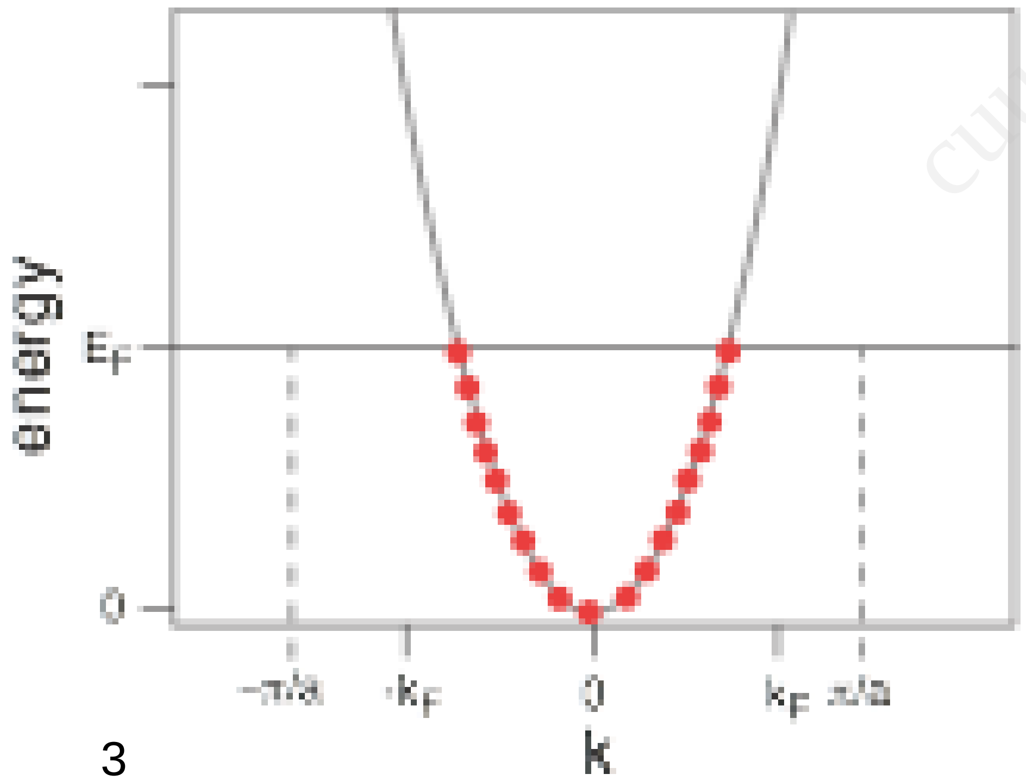
Can we predict this (here in 1D)?



N unit cells -> N possible k values

$$k = \frac{2\pi}{aN} n$$

2 possible states per band and k (spin)

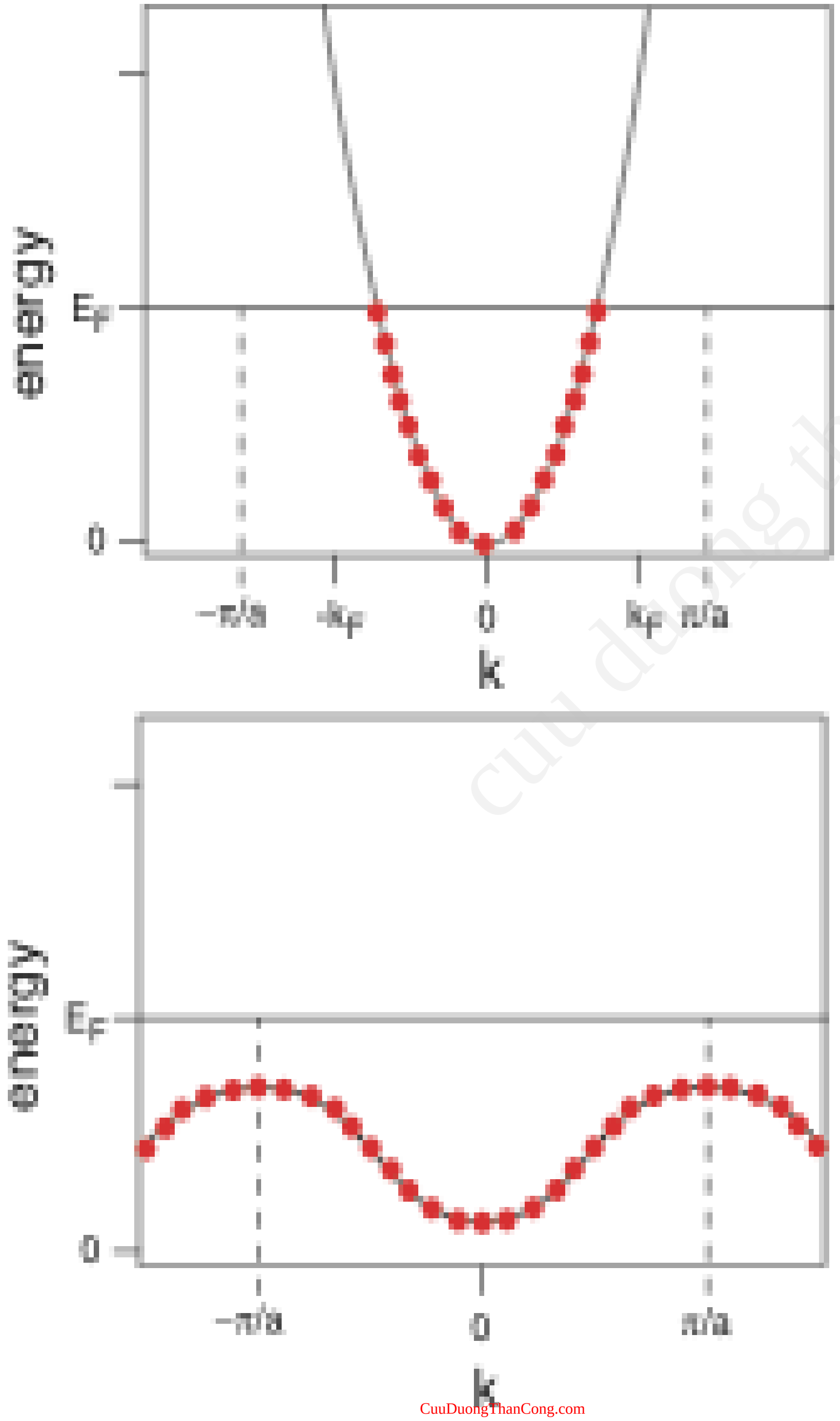


2 valence electrons per unit cell fill one band

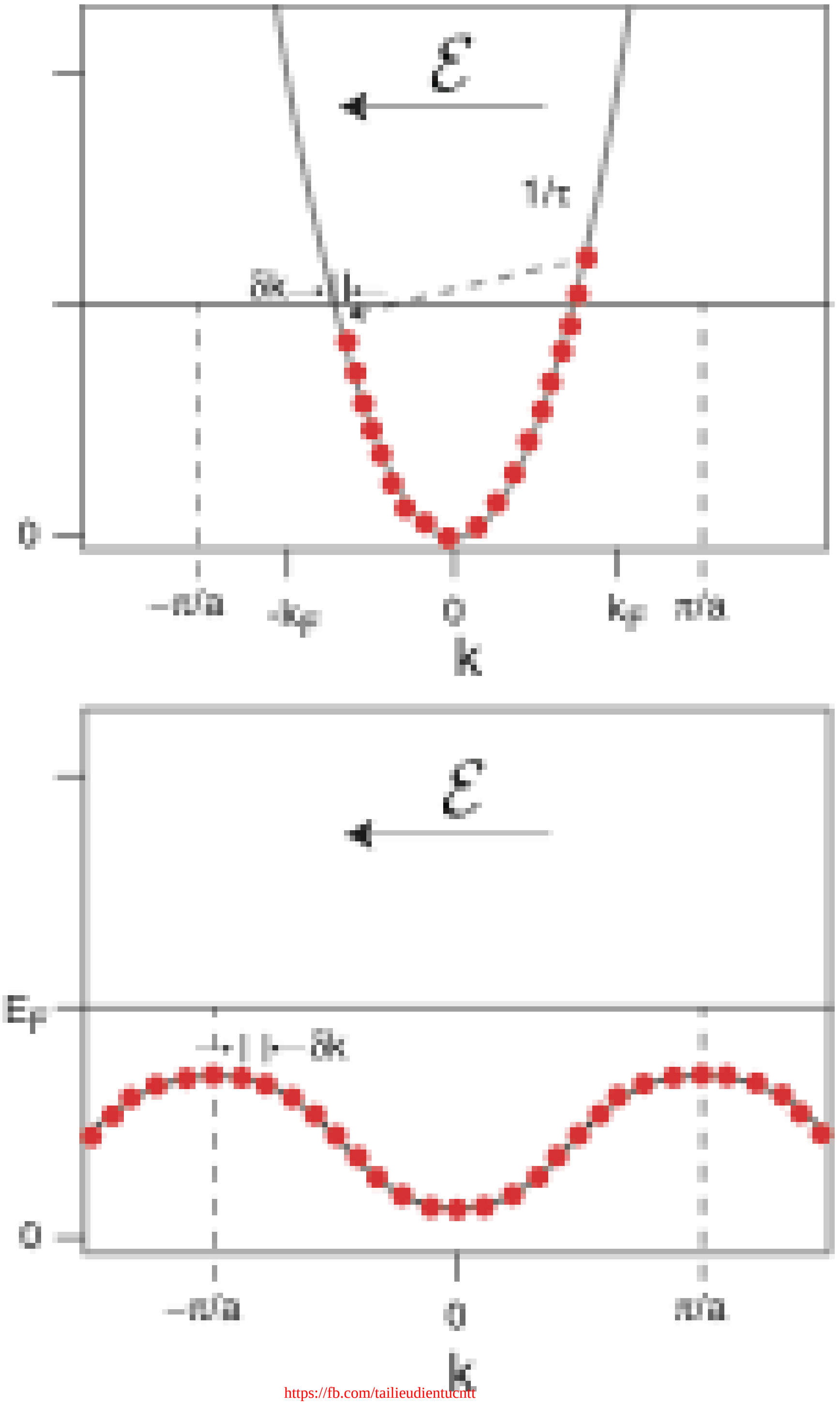
An odd number of valence electrons per unit cell results in a metal equation of motion $$\hbar \frac{dk}{dt} = -e\mathcal{E}.$$

remember also $$v_g = \frac{1}{\hbar}\frac{dE}{dk}$$

no field



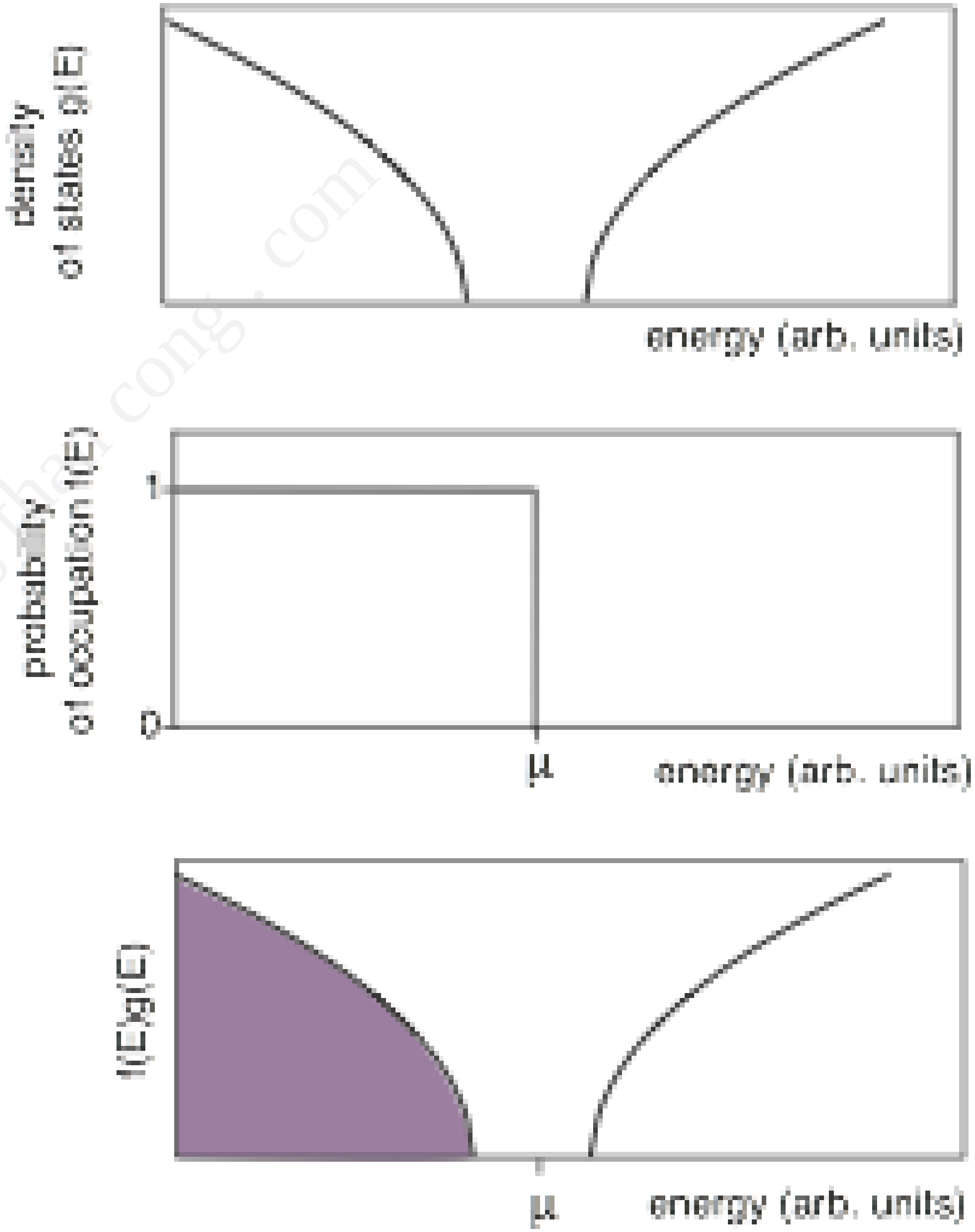
finite field



Can a material with μ in a band gap conduct?

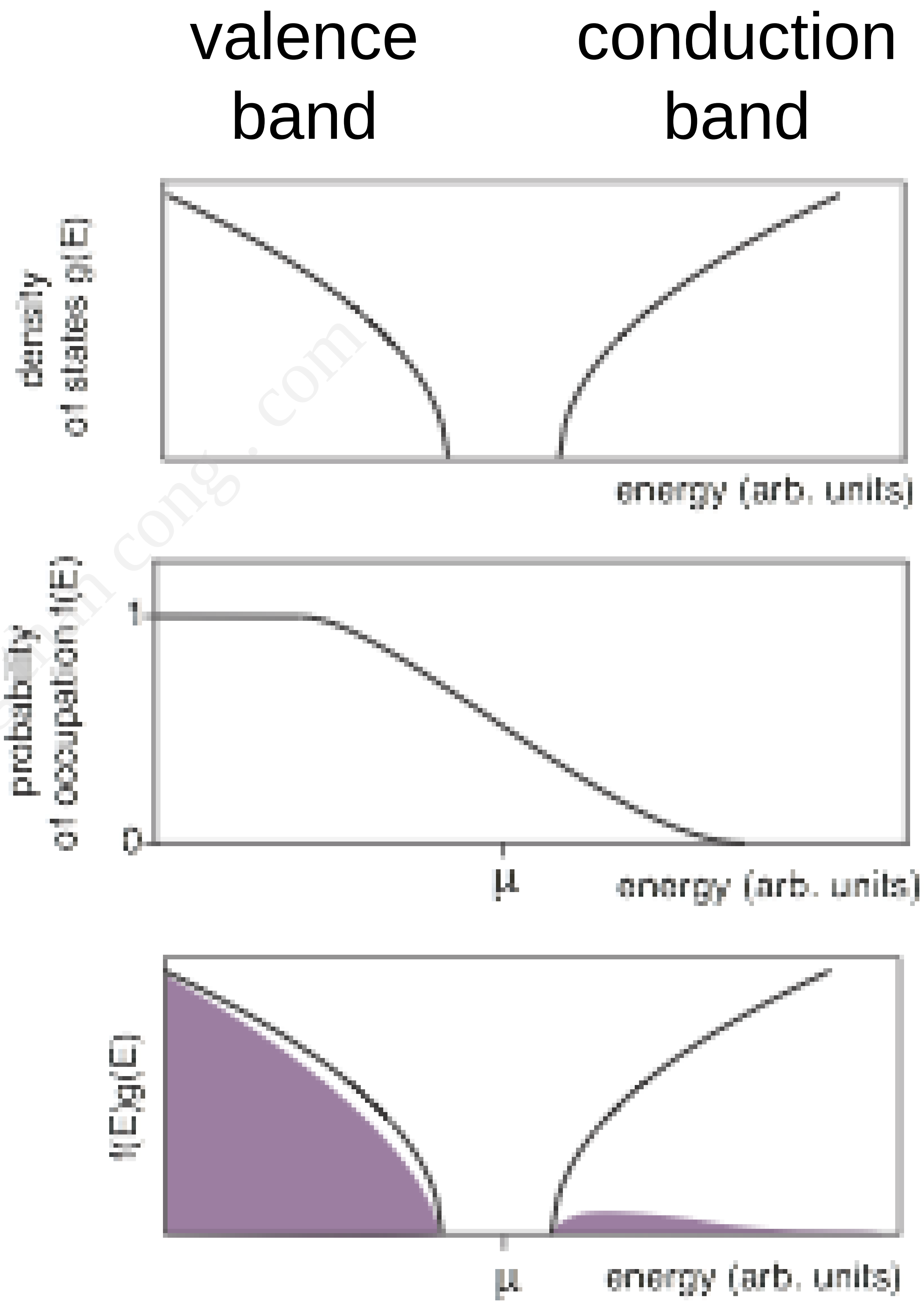
valence band

conduction band



Can a material with μ in a band gap conduct?

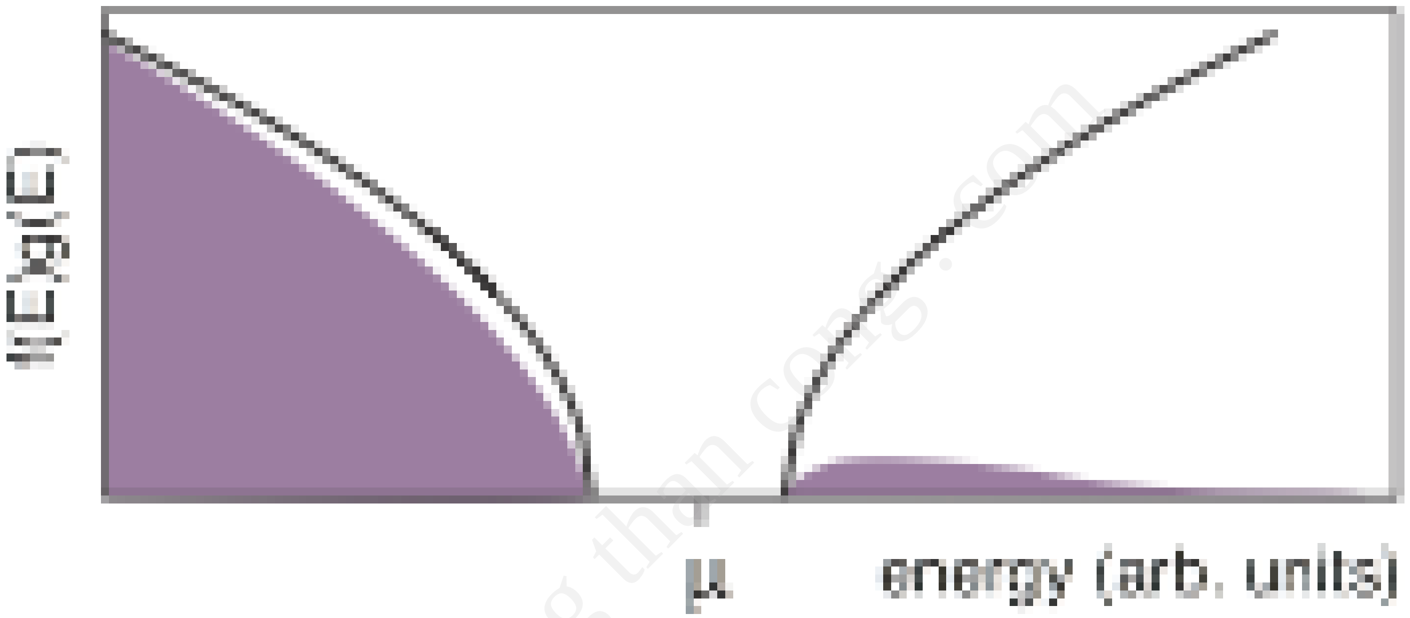
	gap size (eV)
InSb	0.18
InAs	0.36
Ge	0.67
Si	1.11
GaAs	1.43
SiC	2.3
diamond	5.5
MgF_2	11

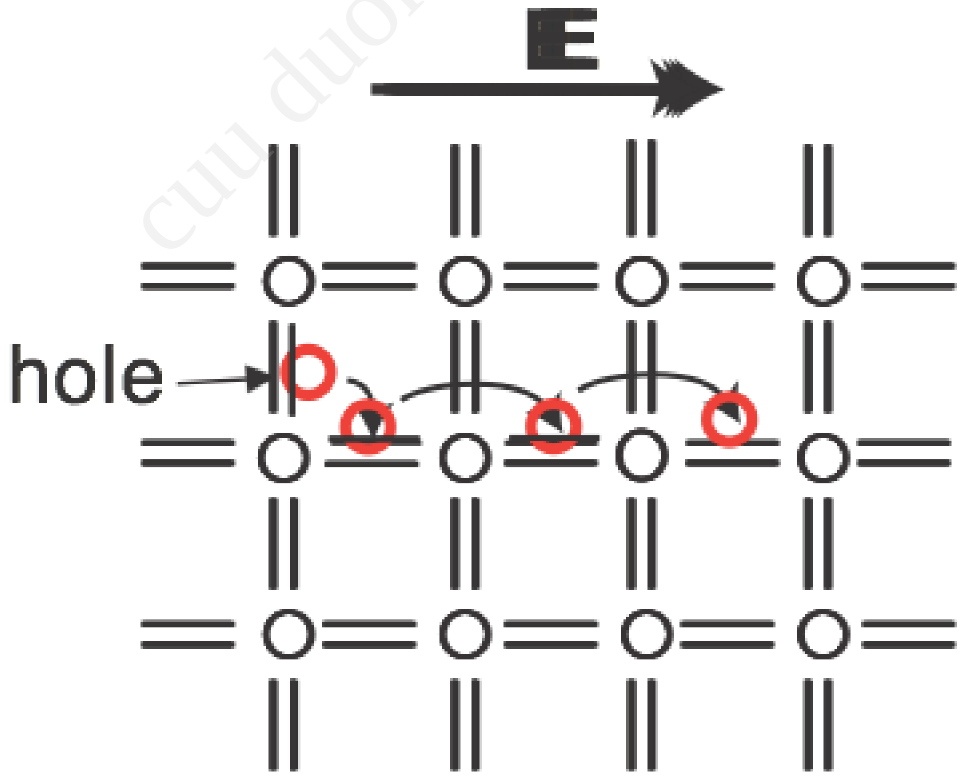


Electrons and holes

valence
band

conduction
band





Intrinsic semiconductors

- Pure, i.e. not doped, semiconductors are called intrinsic.
- For the electronic properties of a semiconductor, “pure” means pure within 1 ppm to 1 ppb.

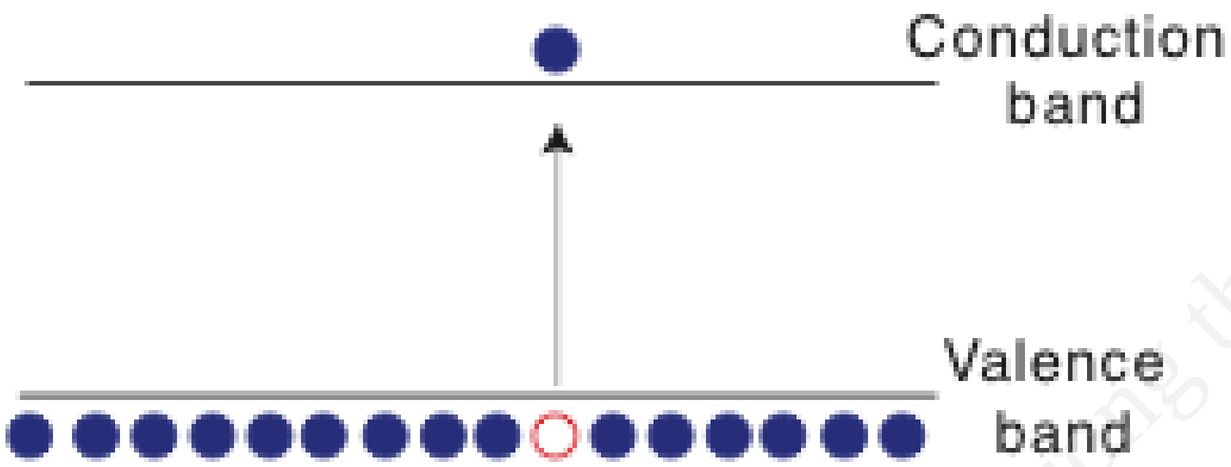
The Fermi-Dirac distribution for a semiconductor

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

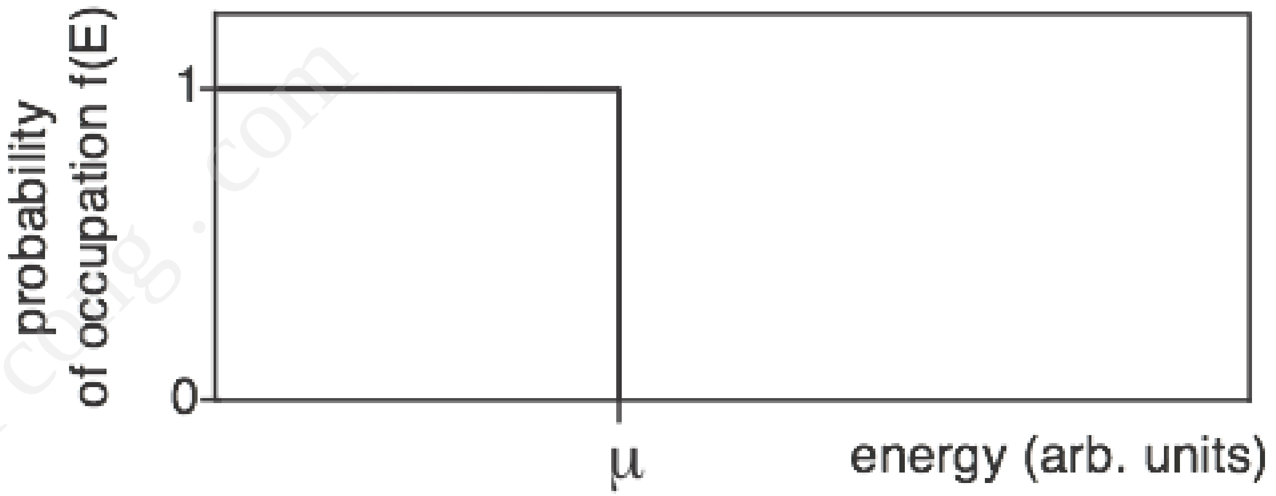
- For a metal, the Fermi energy is the highest occupied energy at 0 K. The chemical potential is temperature-dependent (but not much) and so the two are essentially the same.
- For a semiconductor, the definition of the Fermi energy is not so clear. We better use the chemical potential.
- Some (many) people also use the term “Fermi energy” for semiconductors but then it is temperature-dependent.

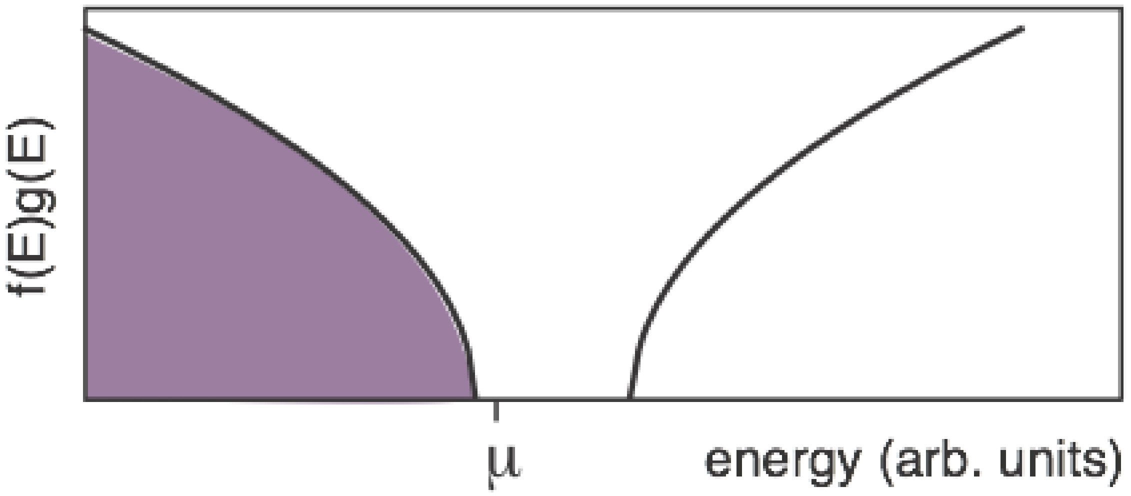
Where is the chemical potential?

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



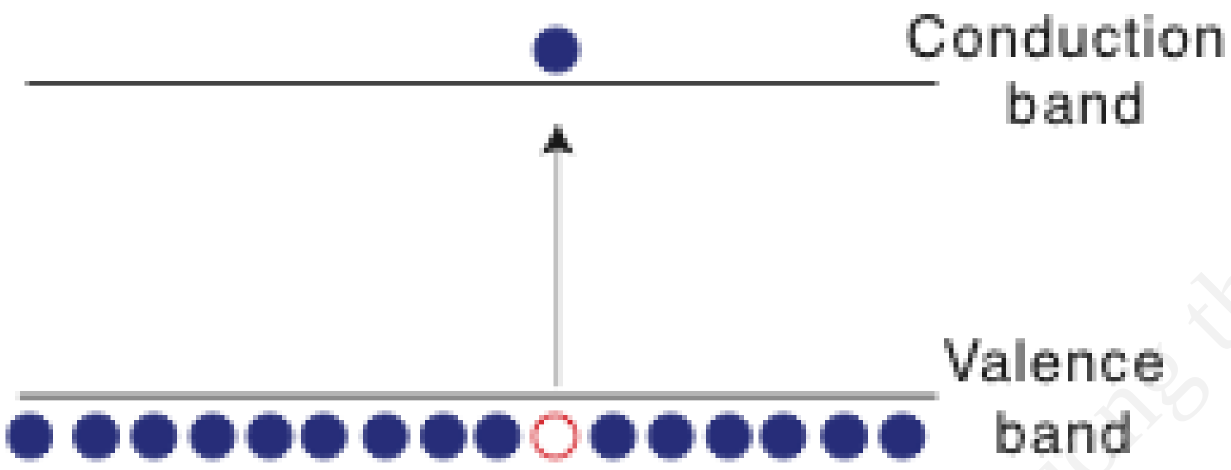
- The chemical potential must be roughly in the middle of the gap. Otherwise one would get an imbalance between conduction electrons than vacant valence states.





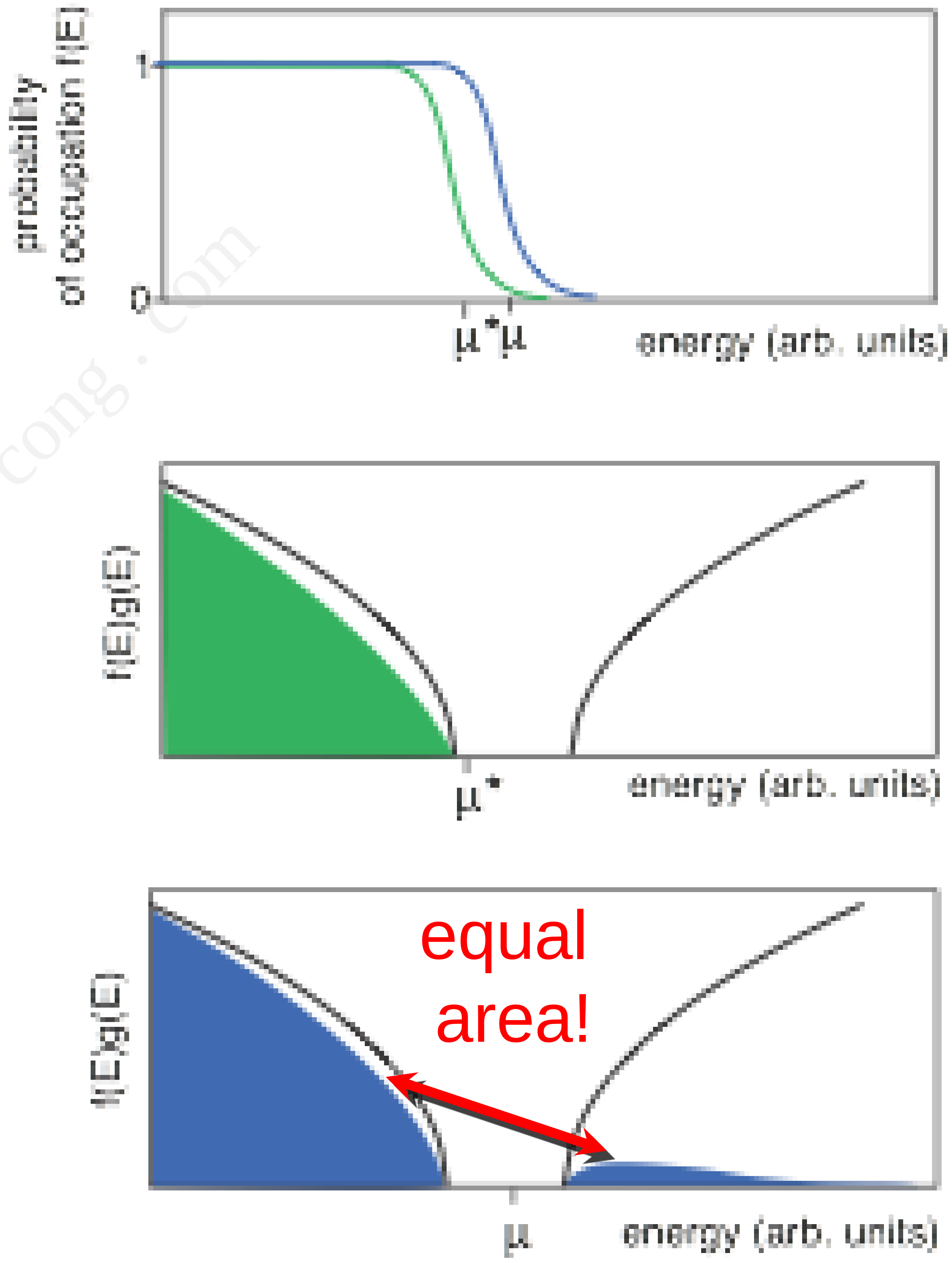
Where is the chemical potential?

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


Conduction band

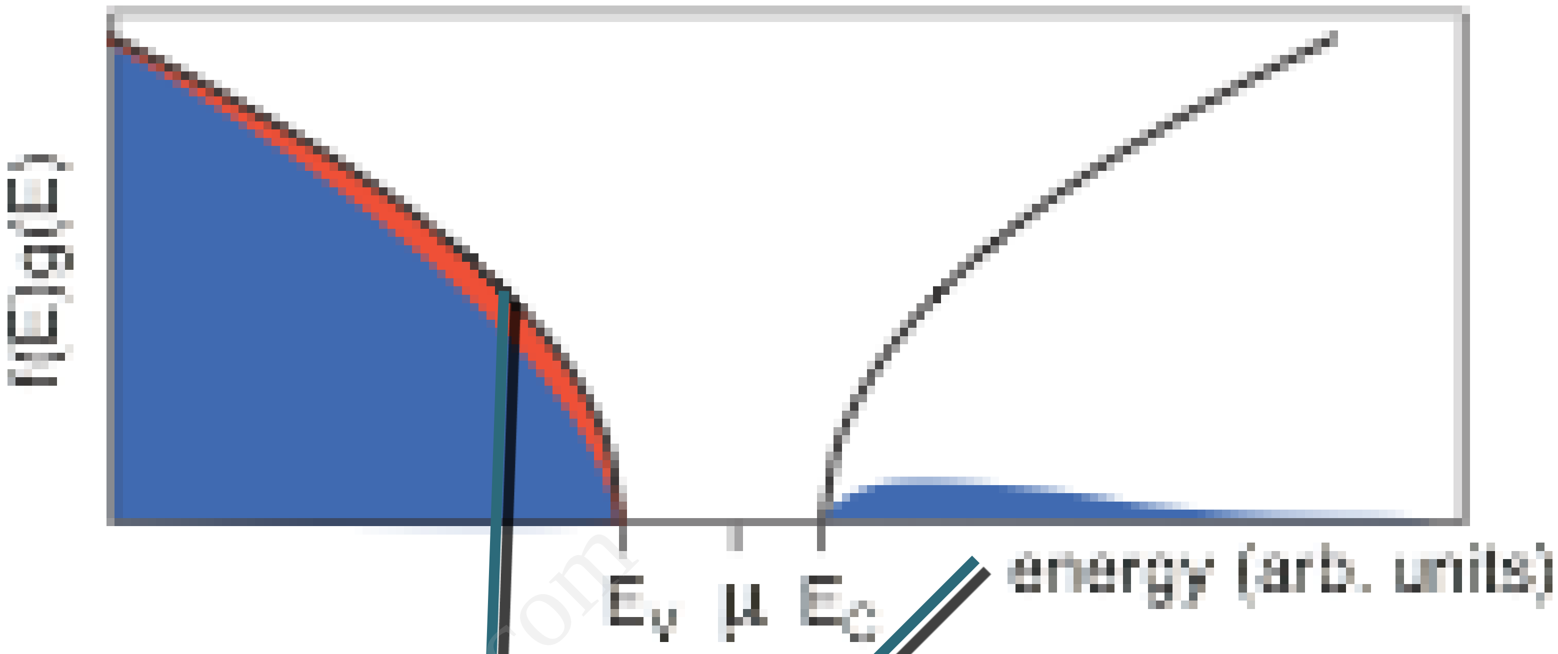
Valence band

- The chemical potential must be roughly in the middle of the gap. Otherwise one would get an imbalance between conduction electrons than vacant valence states.



equal area!

Temperature dependence of the carrier density



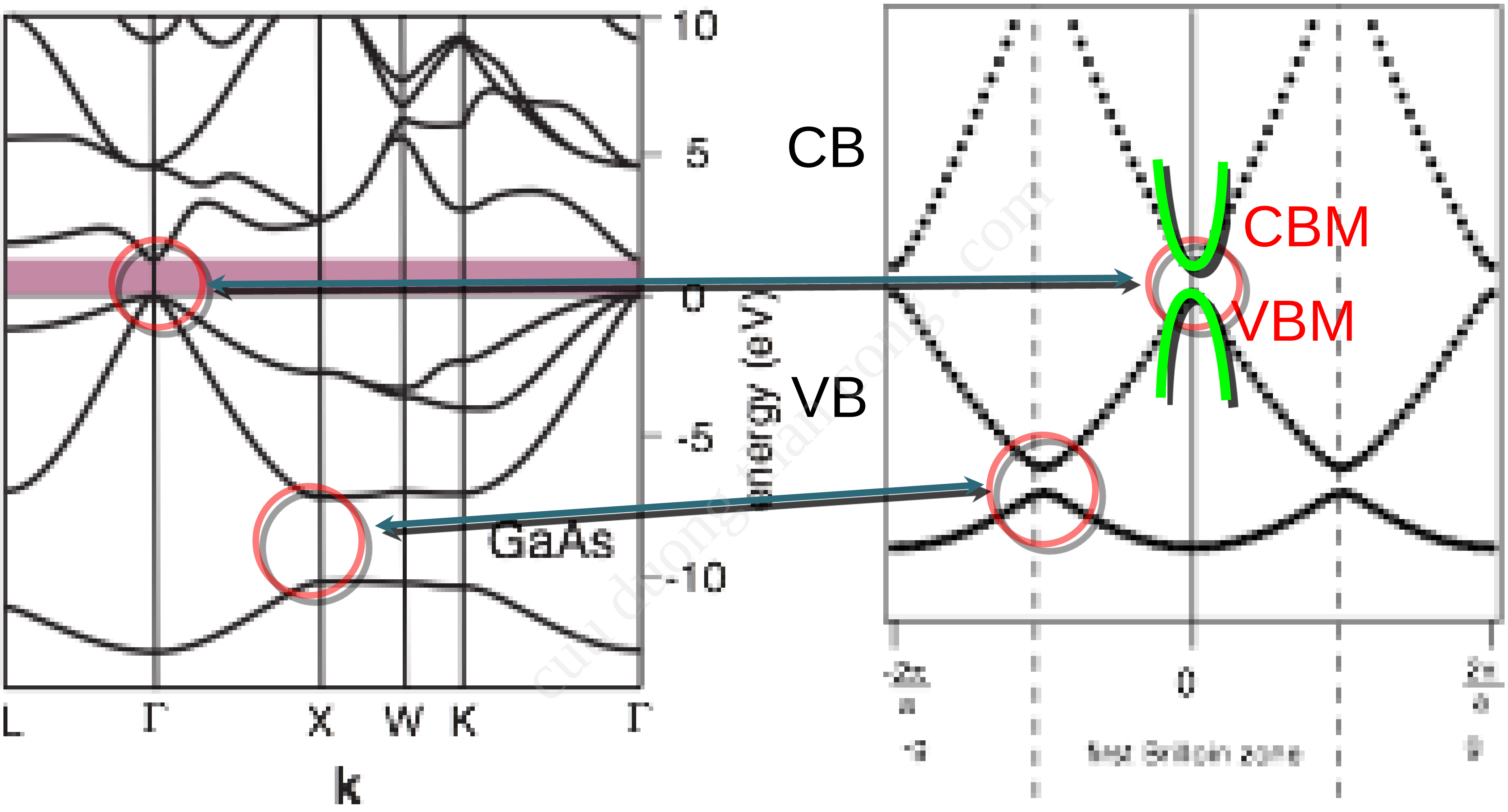
electrons in the conduction band (CB)

$$n = \frac{1}{V}\int_{E_C}^{\infty} g_C(E) f(E,T)\, dE$$

missing electrons (holes) in the valence band (VB)

$$p = \frac{1}{V}\int_{-\infty}^{E_V} g_V(E)[1 - f(E,T)]\, dE$$

Band structures of real materials: Si and GaAs

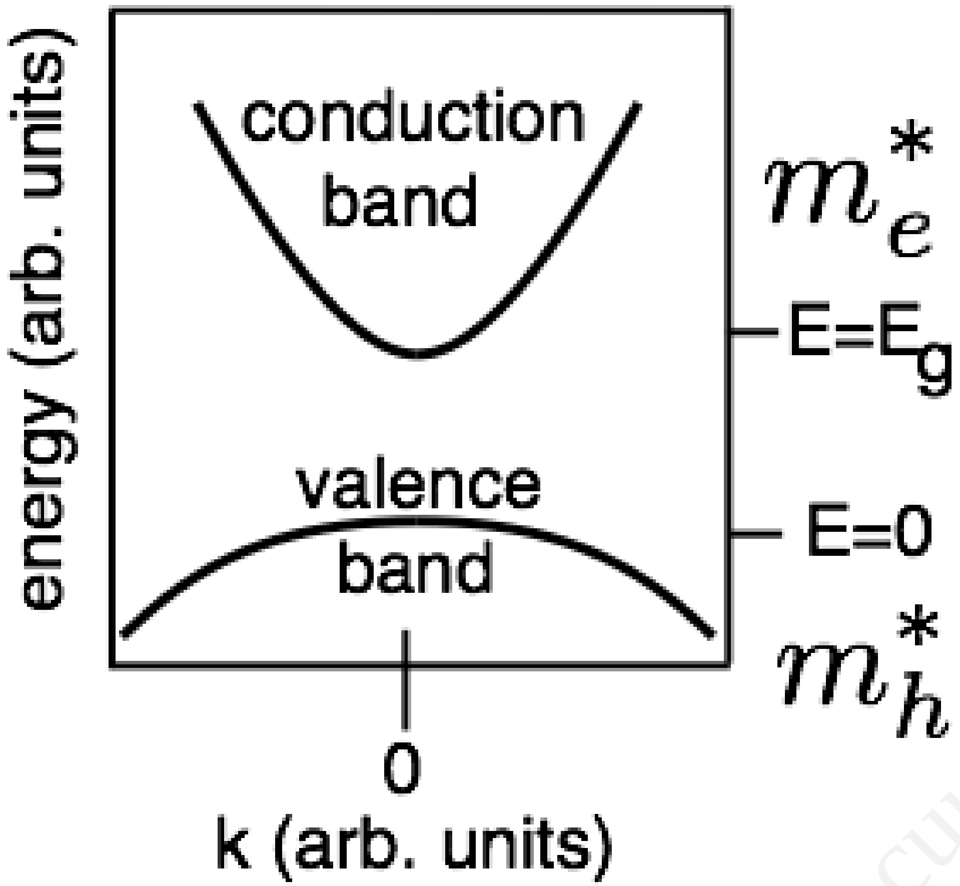


Interpretation

equ. of motion $m^*a = qE$

VB maximum
as E=0

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



conduction band

$q = -e$

$$m^* = \hbar^2 \left(\frac{d^2E(k)}{dk^2} \right)^{-1} > 0$$

A negatively charged particle with a positive mass ("electron")

valence band

$q = -e$ $\quad m^* = \hbar^2 \left(\frac{d^2E(k)}{dk^2} \right)^{-1} < 0$

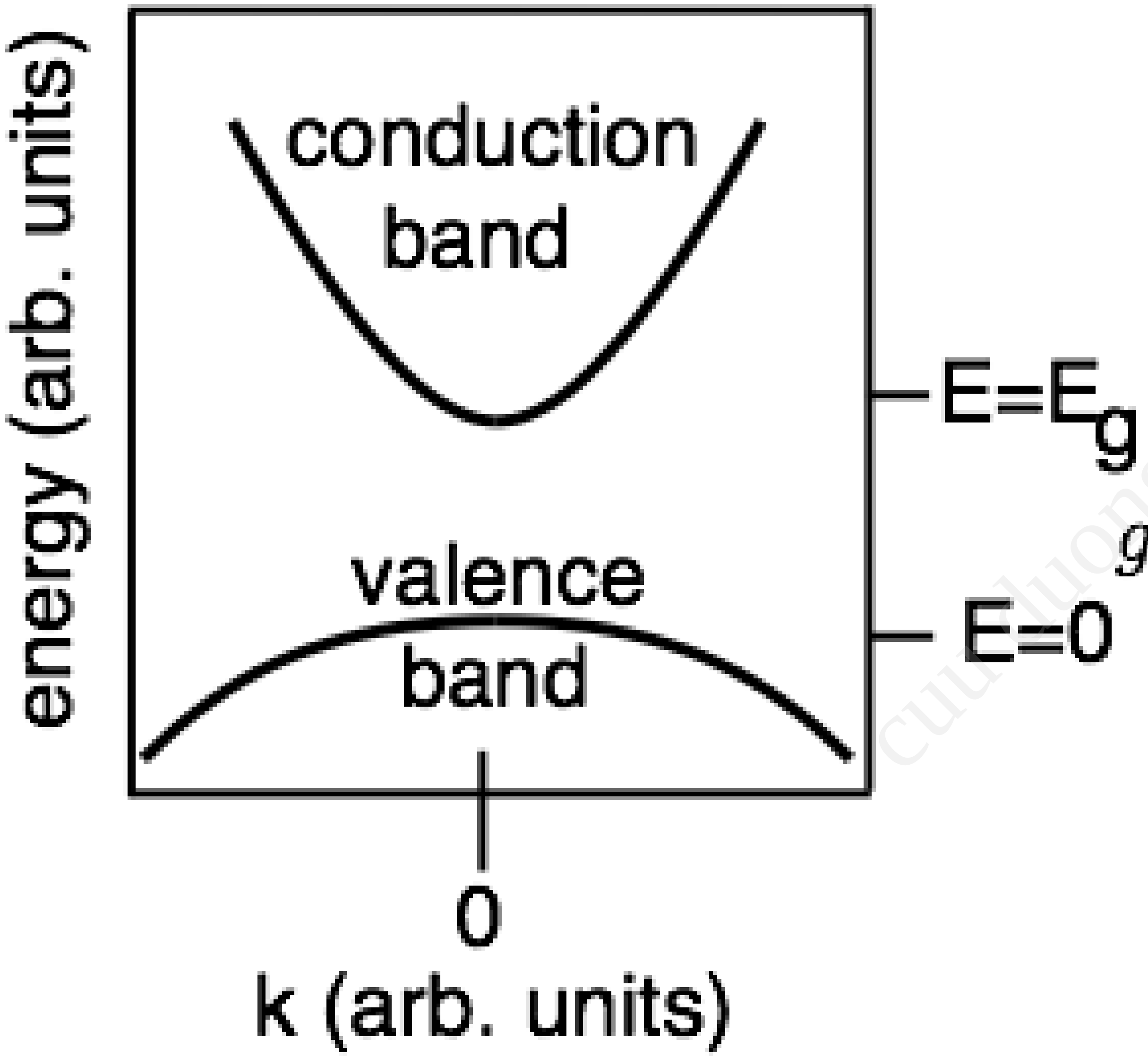
or

$q = e$ $\quad m^* = \hbar^2 \left(\frac{d^2E(k)}{dk^2} \right)^{-1} > 0$

"hole"

Simplified band structure

VB maximum
as E=0



free electrons

$$E(k) = \frac{\hbar^2 k^2}{2m_e}$$

$$g(E)dE = \frac{V}{2\pi^2}\left(\frac{2m_e}{\hbar^2}\right)^{3/2} E^{1/2}dE$$

conduction band

$$E = E_g + \frac{\hbar^2 k^2}{2m_e^*}$$

$$g_C(E)dE = \frac{V}{2\pi^2}\left(\frac{2m_e^*}{\hbar^2}\right)^{3/2} (E - E_g)^{1/2}dE$$

valence band

$$E = -\frac{\hbar^2 k^2}{2m_h^*}$$

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

Temperature dependence of the carrier density

electrons in the conduction band (CB)

$$n = \frac{1}{V}\int_{E_C}^{\infty} g_C(E) f(E,T)\, dE$$

missing electrons (holes) in the valence band (VB)

$$p = \frac{1}{V}\int_{-\infty}^{E_V} g_V(E)[1 - f(E,T)]\, dE$$

Simplified Fermi-Dirac Distribution

for the conduction band $(E-\mu) \gg k_B T$

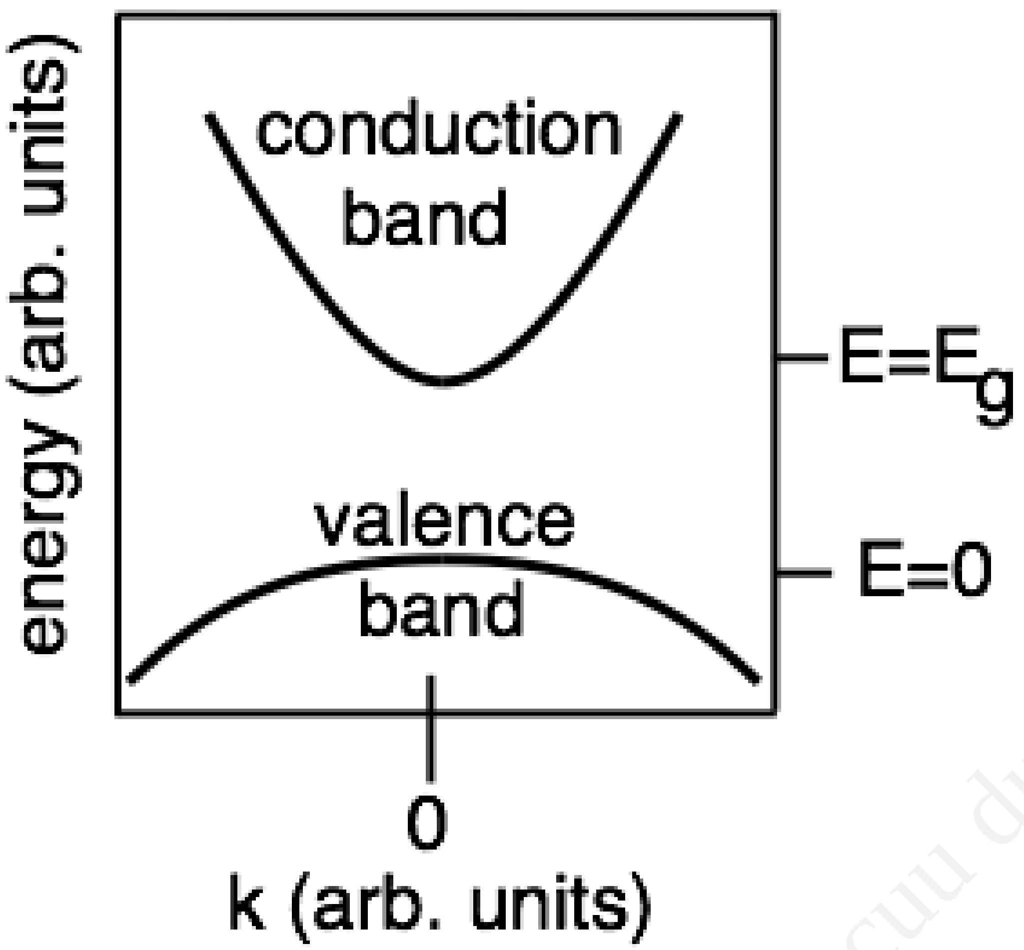
$$f(E,T) = \frac{1}{e^{(E-\mu)/k_B T}+1} \approx e^{-(E-\mu)/k_B T}$$

for the valence band $-(E-\mu) \gg k_B T$

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

Both are Boltzmann distributions!
This is called the non-degenerate case.

The conduction band: occupation



$$g_C(E)dE = \frac{V}{2\pi^2}\left(\frac{2m_e^*}{\hbar^2}\right)^{3/2}(E-E_g)^{1/2}dE$$

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

$$n = \frac{1}{V}\int_{E_g}^{\infty}\frac{V}{2\pi^2}\left(\frac{2m_e^*}{\hbar^2}\right)^{3/2}(E-E_g)^{1/2}e^{-(E-\mu)/k_BT}dE$$

$$= \frac{(2m_e^*)^{3/2}}{2\pi^2\hbar^3}e^{\mu/k_BT}\int_{E_g}^{\infty}(E-E_g)^{1/2}e^{-E/k_BT}dE$$

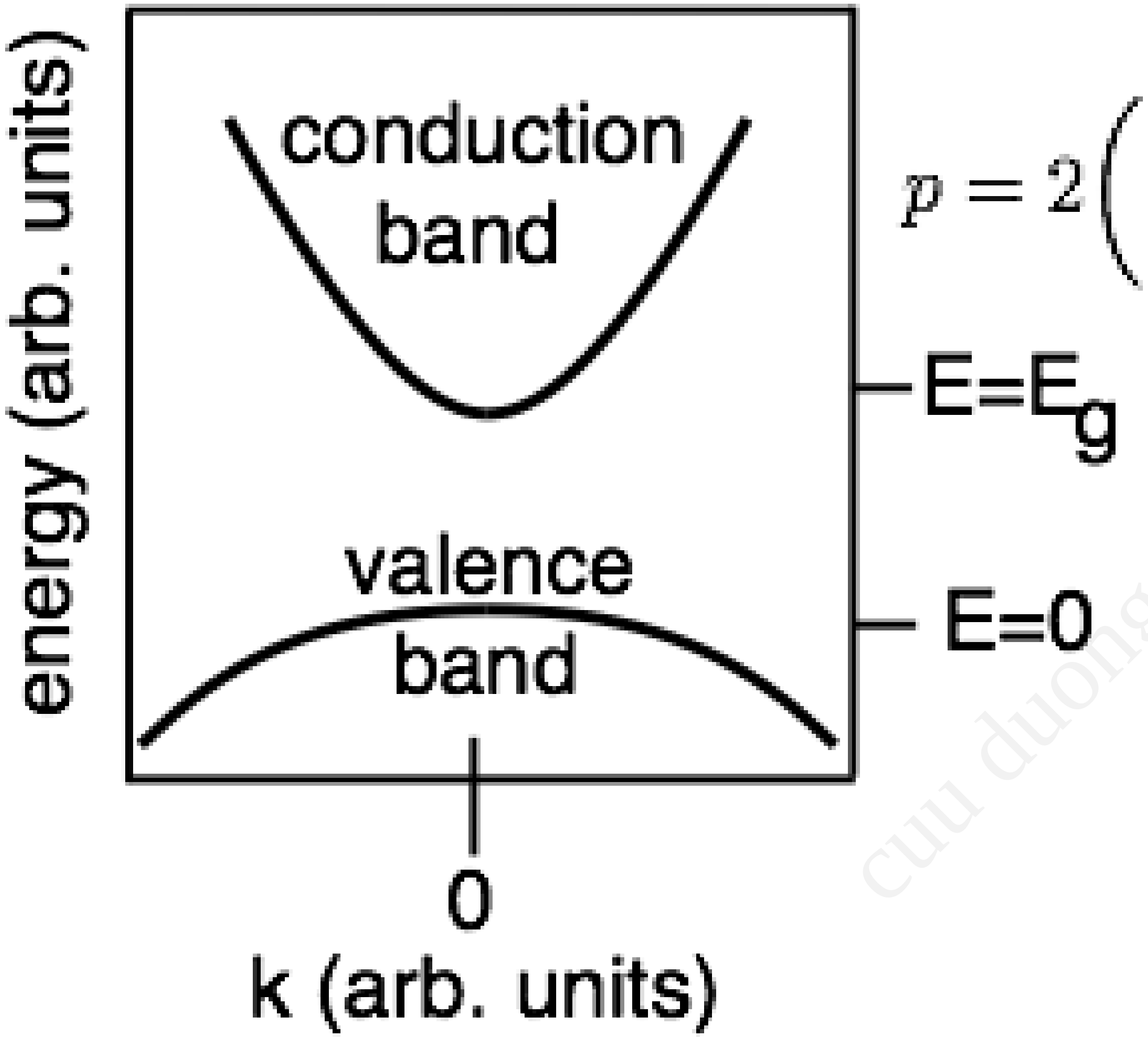
substitution $X_g = (E-E_g)/k_BT$

$$n = \frac{(2m_e^*)^{3/2}}{2\pi^2\hbar^3}(k_BT)^{3/2}e^{-(E_g-\mu)/k_BT}\int_0^{\infty}X_g^{1/2}e^{-X_g}dX_g$$

$\sqrt{\pi}/2$

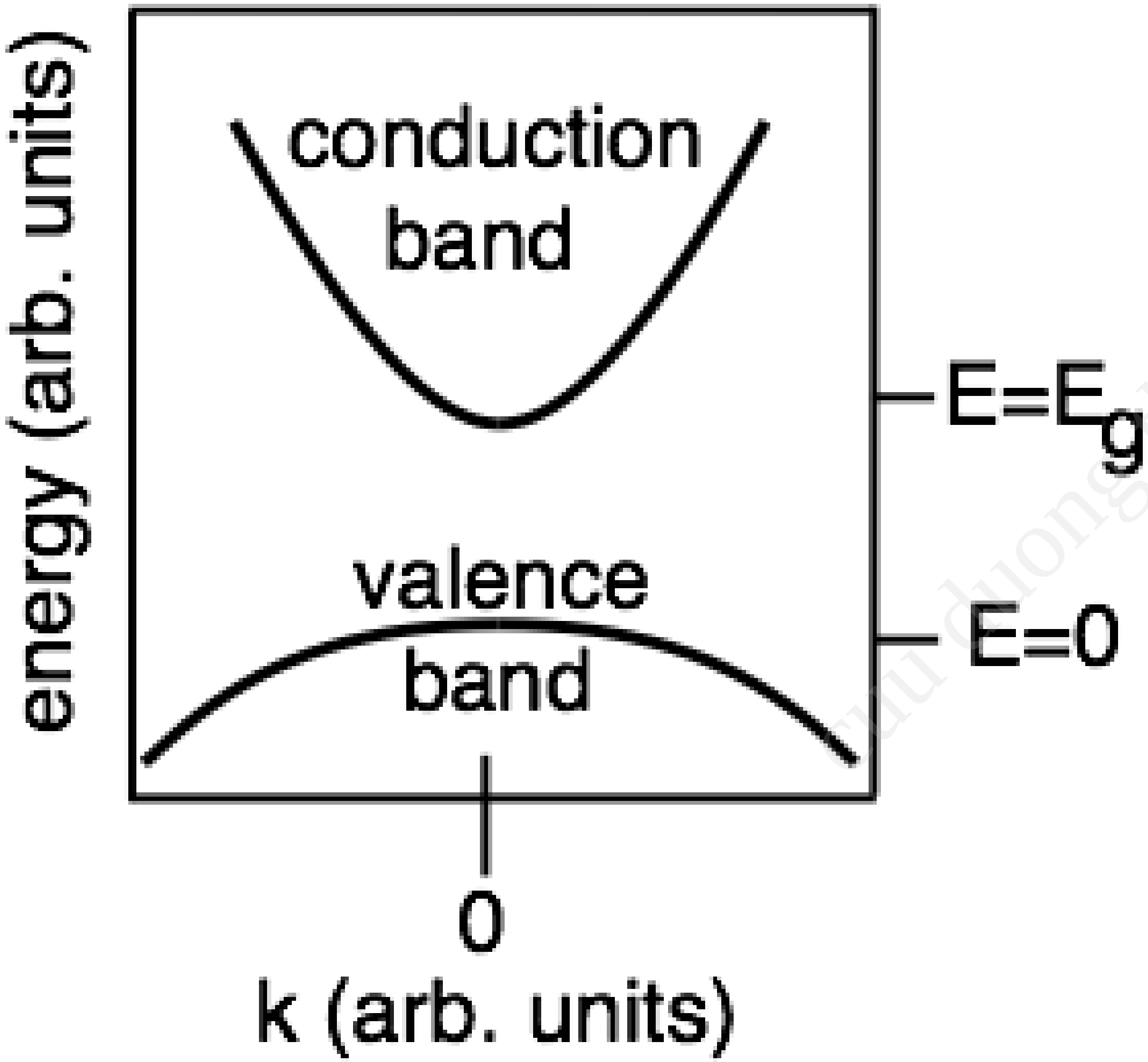
$$n = 2\left(\frac{2\pi m_e^* k_BT}{h^2}\right)^{3/2}e^{-(E_g-\mu)/k_BT} = N_{\text{eff}}^{C}e^{-(E_g-\mu)/k_BT}$$

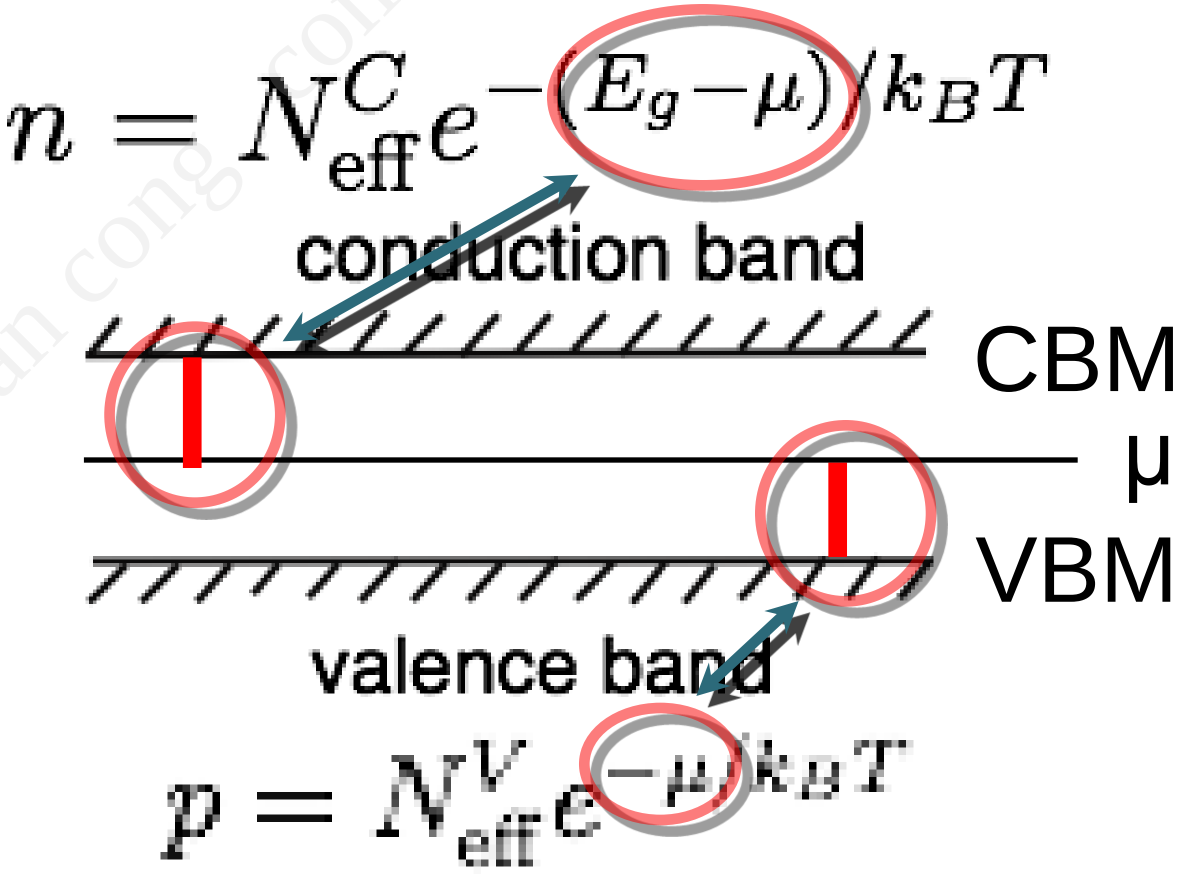
The valence band: occupation



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

The valence band: occupation





$$n = N_{\text{eff}}^{C} e^{-(E_g-\mu)/k_B T}$$

$$p = N_{\text{eff}}^{V} e^{-\mu/k_B T}$$

Law of mass action

$$n = 2\left(\frac{2\pi m_e^* k_B T}{h^2}\right)^{3/2} e^{-(E_g-\mu)/k_BT} = N_{\text{eff}}^C e^{-(E_g-\mu)/k_BT} \qquad p = 2\left(\frac{2\pi m_h^* k_B T}{h^2}\right)^{3/2} e^{-\mu/k_BT} = N_{\text{eff}}^V e^{-\mu/k_BT}$$

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

This does not depend on the position of μ.

and finally with $n_i = p_i$

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

Example

$$n = N_{\text{eff}}^{C} e^{-(E_g-\mu)/k_BT} = N_{\text{eff}}^{C} e^{-E_g/2k_BT}$$

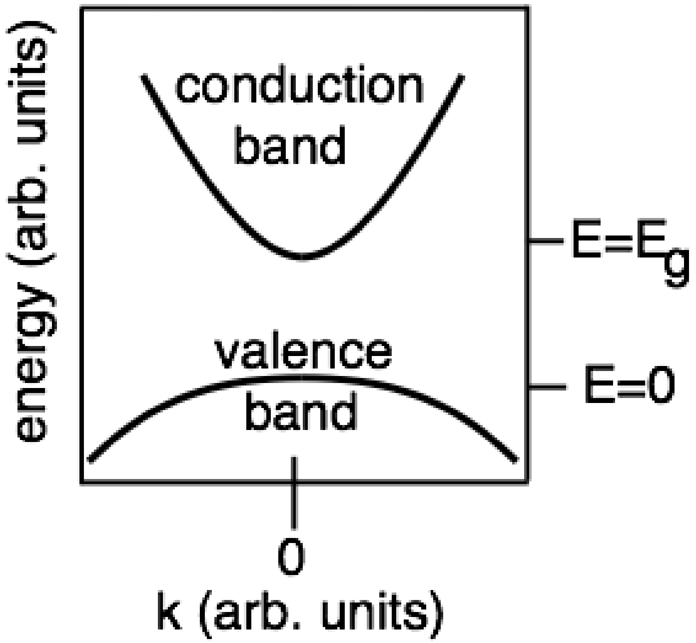
$$N_{\text{eff}}^{C} = 10^{25}\text{m}^{-3}$$

	gap size (eV)	n in m^{-3} at 150 K	n in m^{-3} at 300 K
InSb	0.18	$2\text{x}10^{22}$	$6\text{x}10^{23}$
Si	1.11	$4\text{x}10^{6}$	$2\text{x}10^{16}$
diamond	5.5	$6\text{x}10^{-68}$	$1\text{x}10^{-21}$

Where is μ?

$$n = p$$

$$n = 2\left(\frac{2\pi m_e^* k_B T}{h^2}\right)^{3/2} e^{-(E_g-\mu)/k_BT} = N_{\text{eff}}^C e^{-(E_g-\mu)/k_BT} \qquad p = 2\left(\frac{2\pi m_h^* k_B T}{h^2}\right)^{3/2} e^{-\mu/k_BT} = N_{\text{eff}}^V e^{-\mu/k_BT}$$



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

These are the parameters one needs to know.

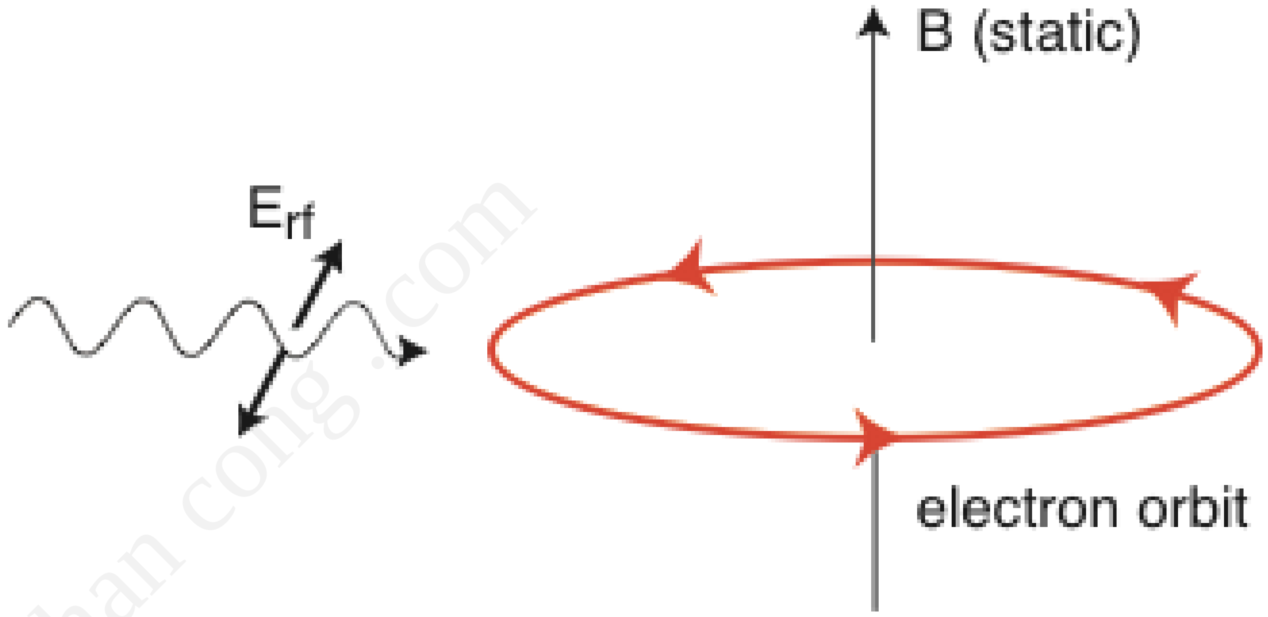
effective mass from conductivity?

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

The cyclotron effective mass

$$m\omega^2 r = e\frac{2\pi r}{T}B = e\omega r B$$

$$\omega_c = \frac{Be}{m_e^*}$$

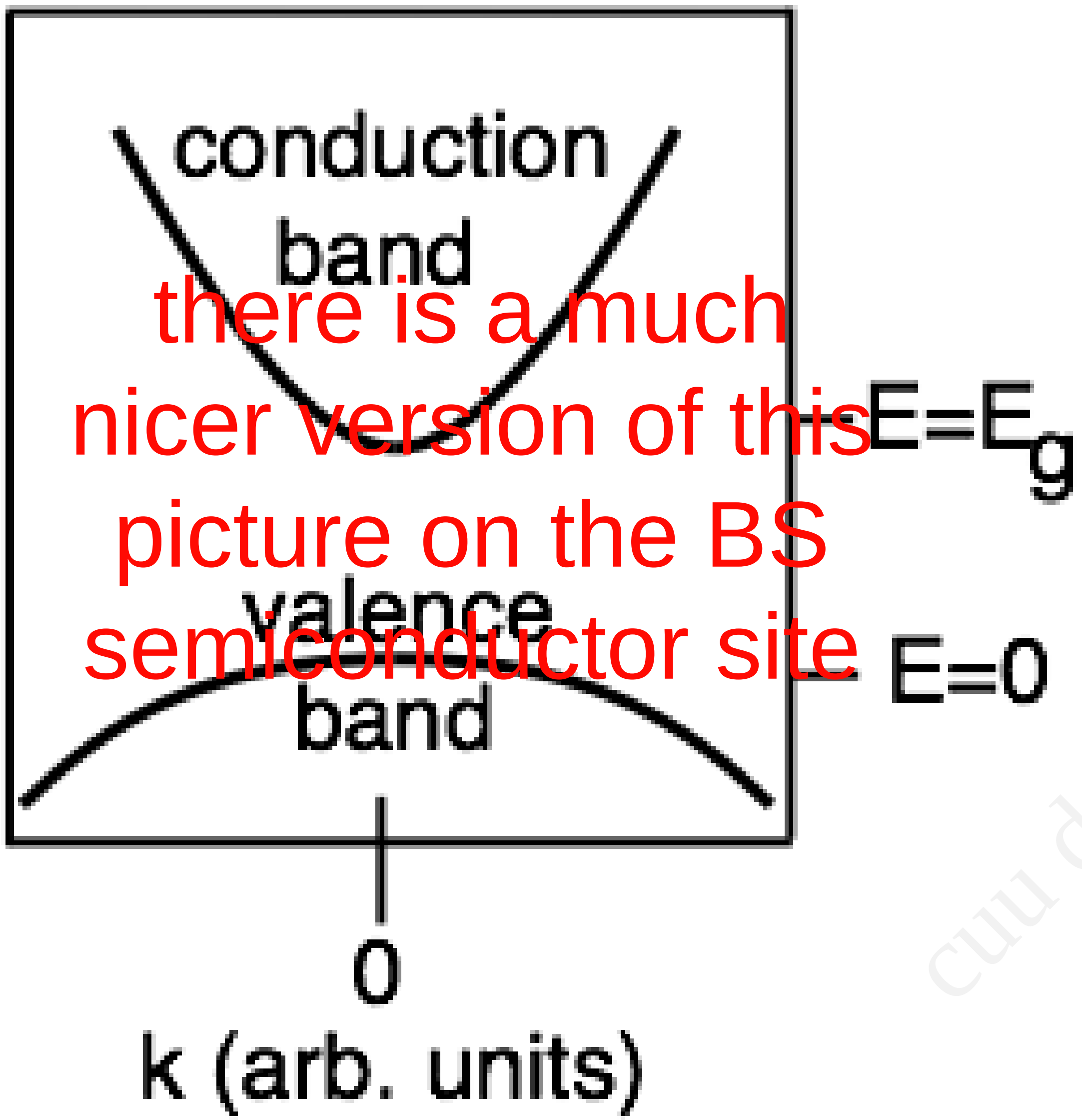


quantized levels $E = E_0 + (n + \frac{1}{2})\hbar\omega_C$

resonant absorption of the radio frequency signal at ω_c

Absorption works because there are actually many (so called Landau) levels with an energy separation of $\hbar\omega_C$

The effective mass



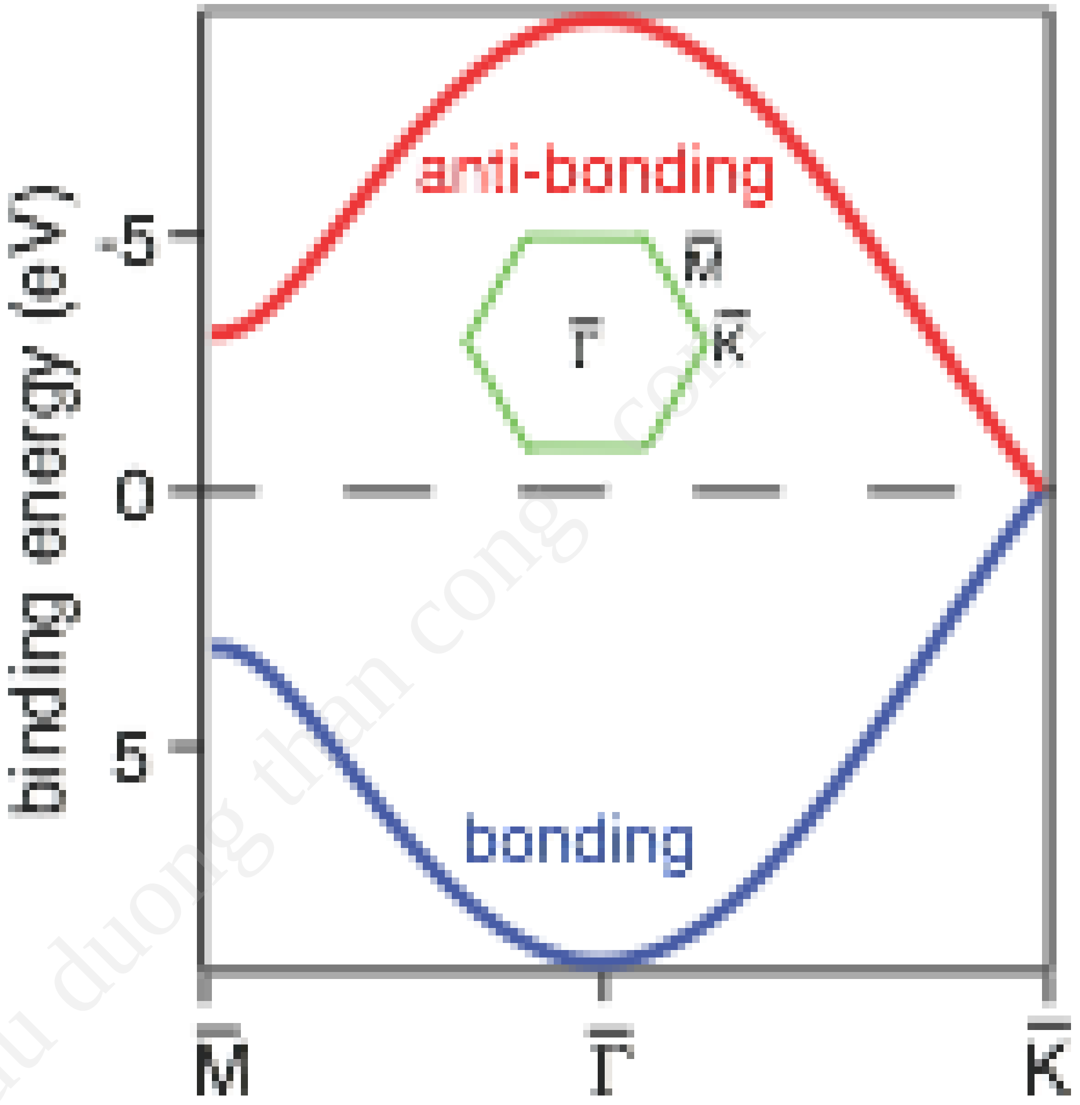
there is a much nicer version of this picture on the BS semiconductor site

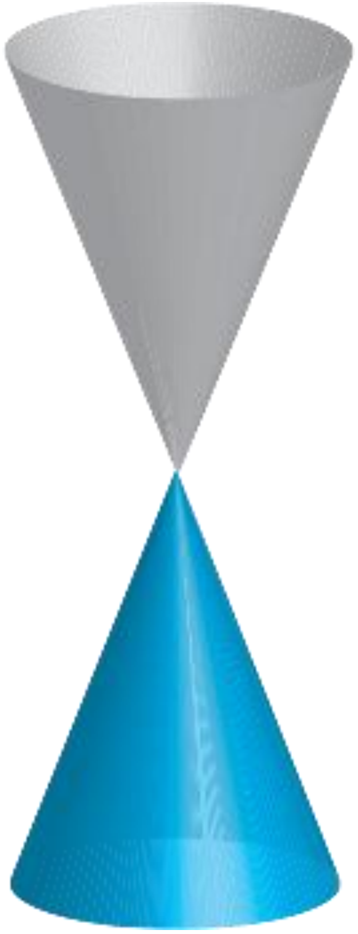
	m_e^*/m_e	m_h^*/m_e
InSb	0.014	0.4
InAs	0.022	0.4
Ge	0.6	0.28
Si	0.43	0.54
GaAs	0.065	0.5
Na	1.2	
Cu	0.99	
Sb	0.85	

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

relativistic and massless??

- relativistic physics with “slow” electrons?
- the usual definition of the effective mass does not give 0!



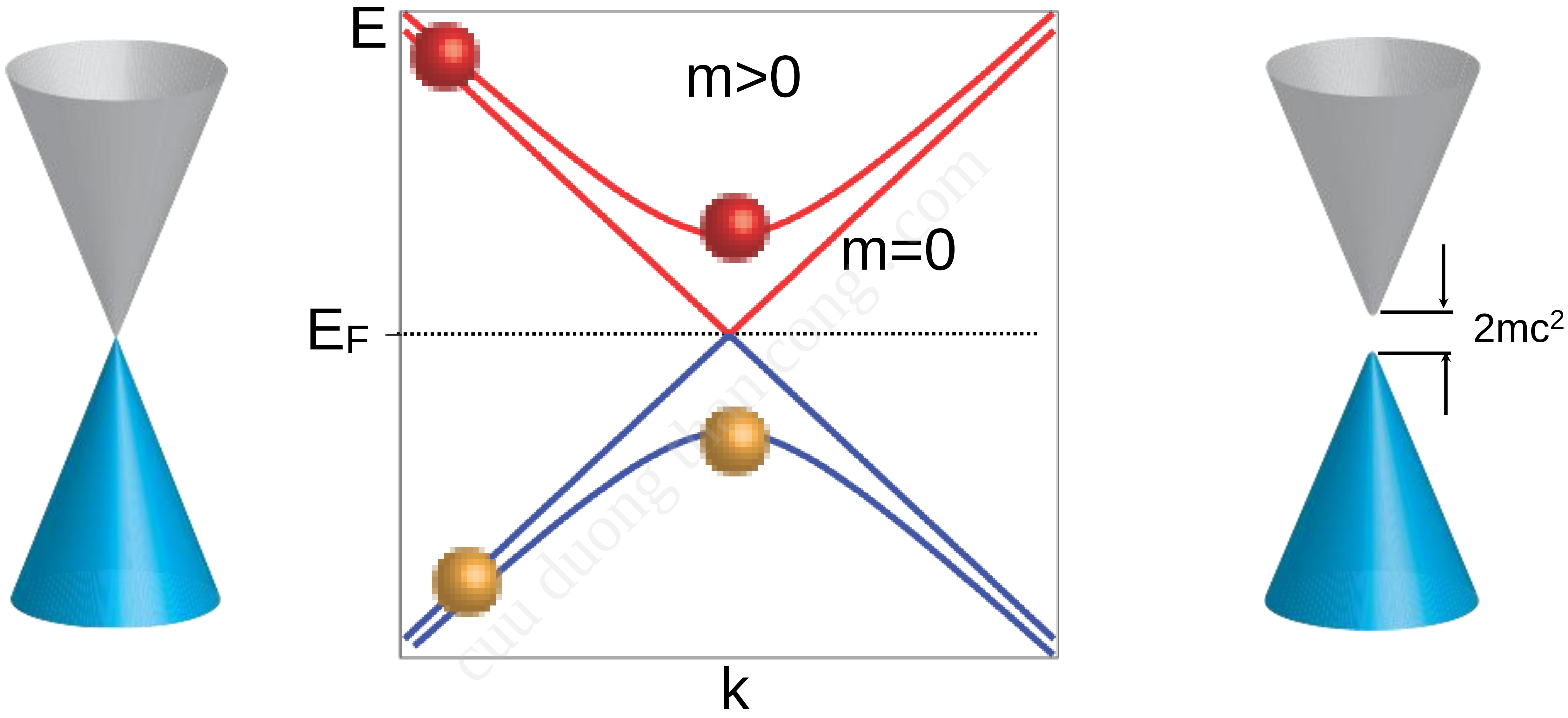


usually

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

massless / semimetal

massive / semiconductor



$$E = \pm pc = \pm \hbar k c$$

$$E = \pm\sqrt{(mc^2)^2 + (pc)^2}$$

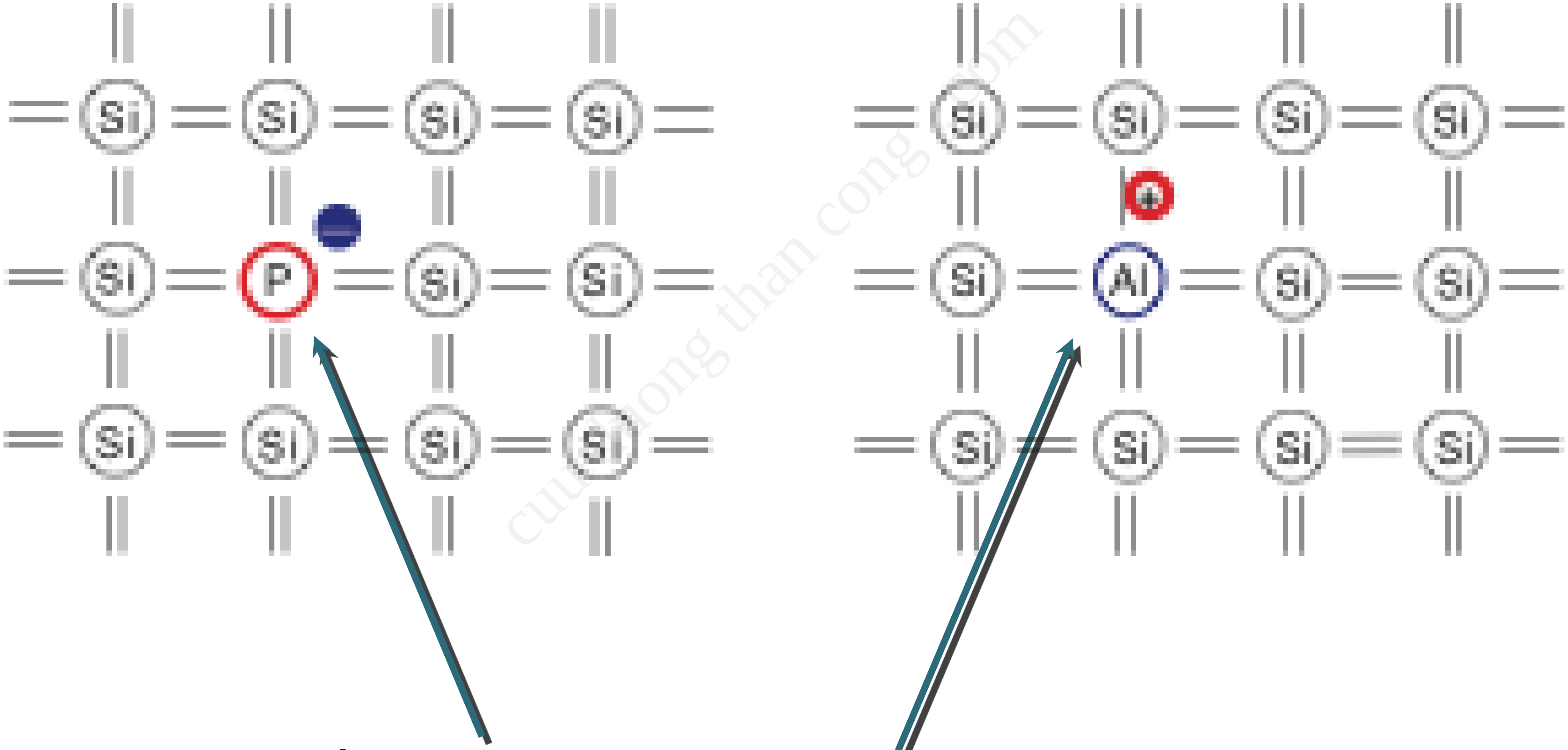
● electron

● hole

Doped semiconductors

- A **very small** amount of impurities can have a big influence on the conductivity of a semiconductor.
- Controlled addition of impurities is called doping.
- There are two types of doping: *n* doping (impurities increasing #electrons) and *p* doping (impurities increasing #of holes).
- Typical doping levels are in the order of 10^{19} to 10^{23} impurity atoms per m^3. Remember: Si has a concentration of $5*10^{28}$ atoms per m^3 and an intrinsic carrier concentration of 10^{16} electrons/holes per m^3 at room temperature.

n- and *p*-doping

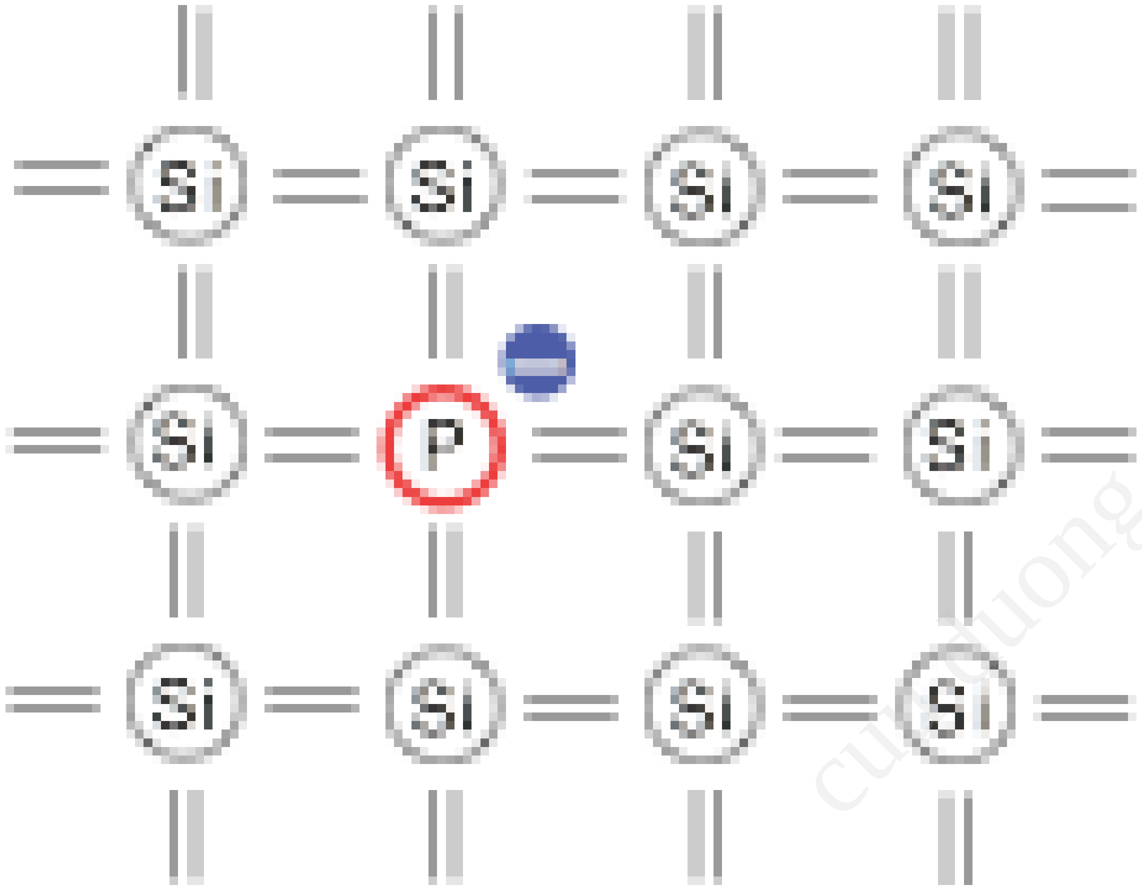


donor atom

acceptor atom

n-doping

phosphorus
penta-valent,
one electron too many



Estimate binding energy with Bohr model:

$$E_n = -\frac{m_e e^4}{8\epsilon_0^2 h^2}\frac{1}{n^2}$$

using the modifications

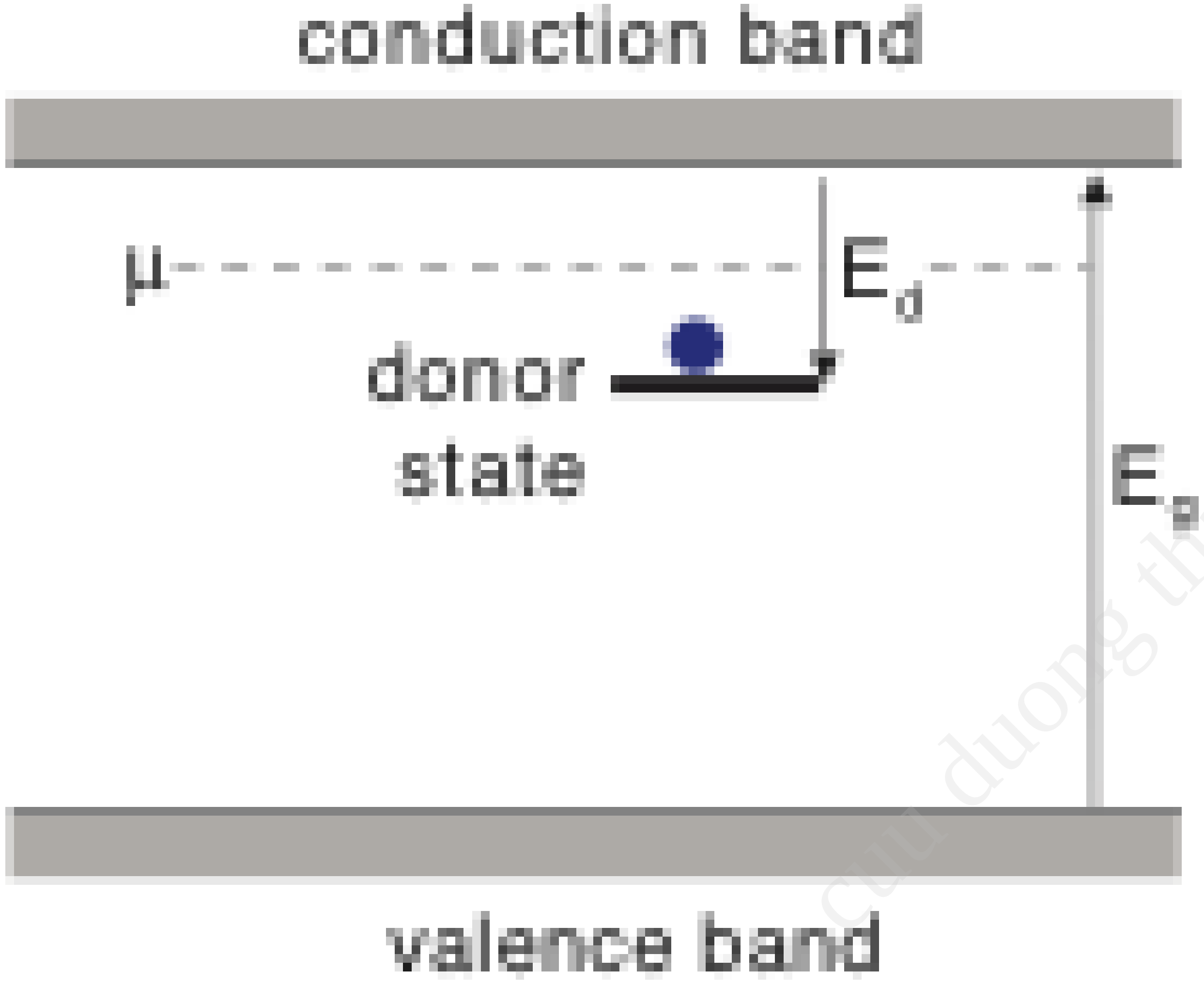
$$m_e \rightarrow m^* \approx 0.43 m_e$$

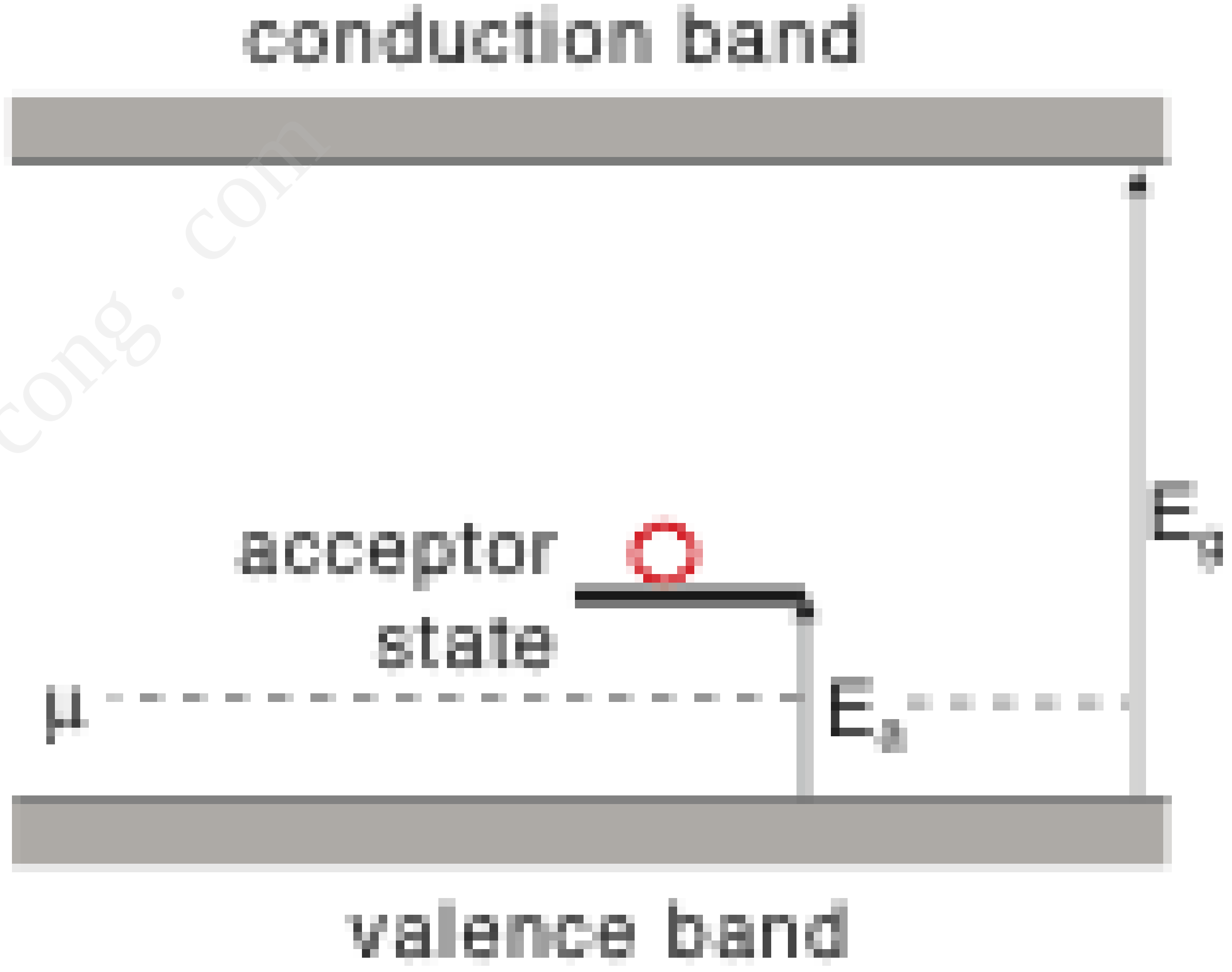
$$\epsilon_0 \rightarrow \epsilon\epsilon_0 \approx 11.7\epsilon_0$$

order of magnitude

$$E_1 = -30 \text{ meV}$$

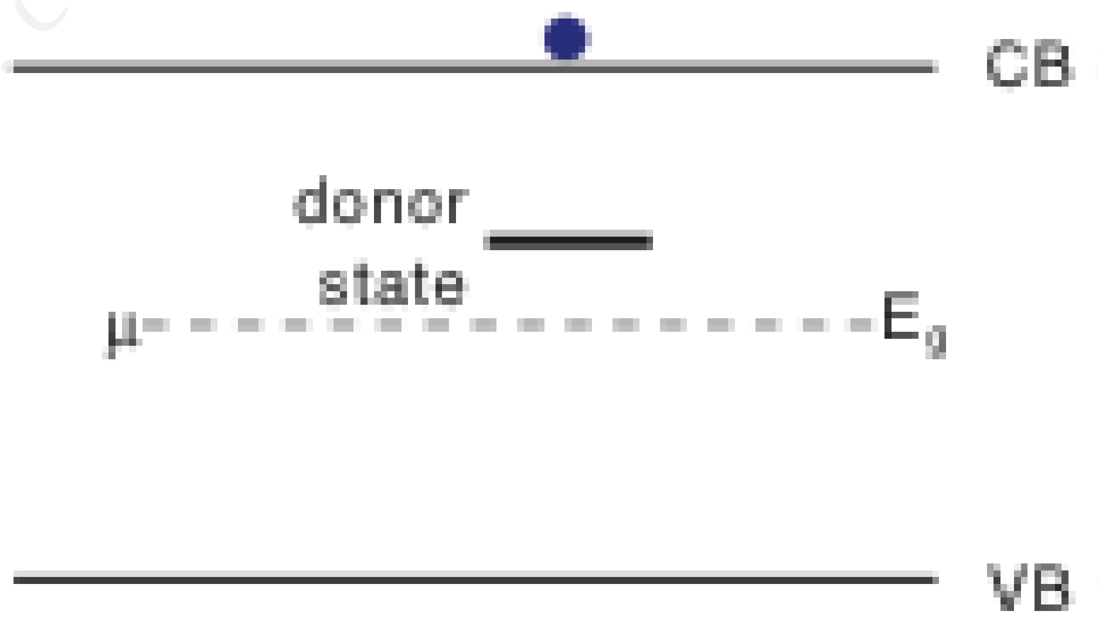
$$a_0 = \frac{4\pi\epsilon_0 \hbar^2}{m_e e^2}$$


conduction band
μ
E
d
donor
state
E
g
valence band

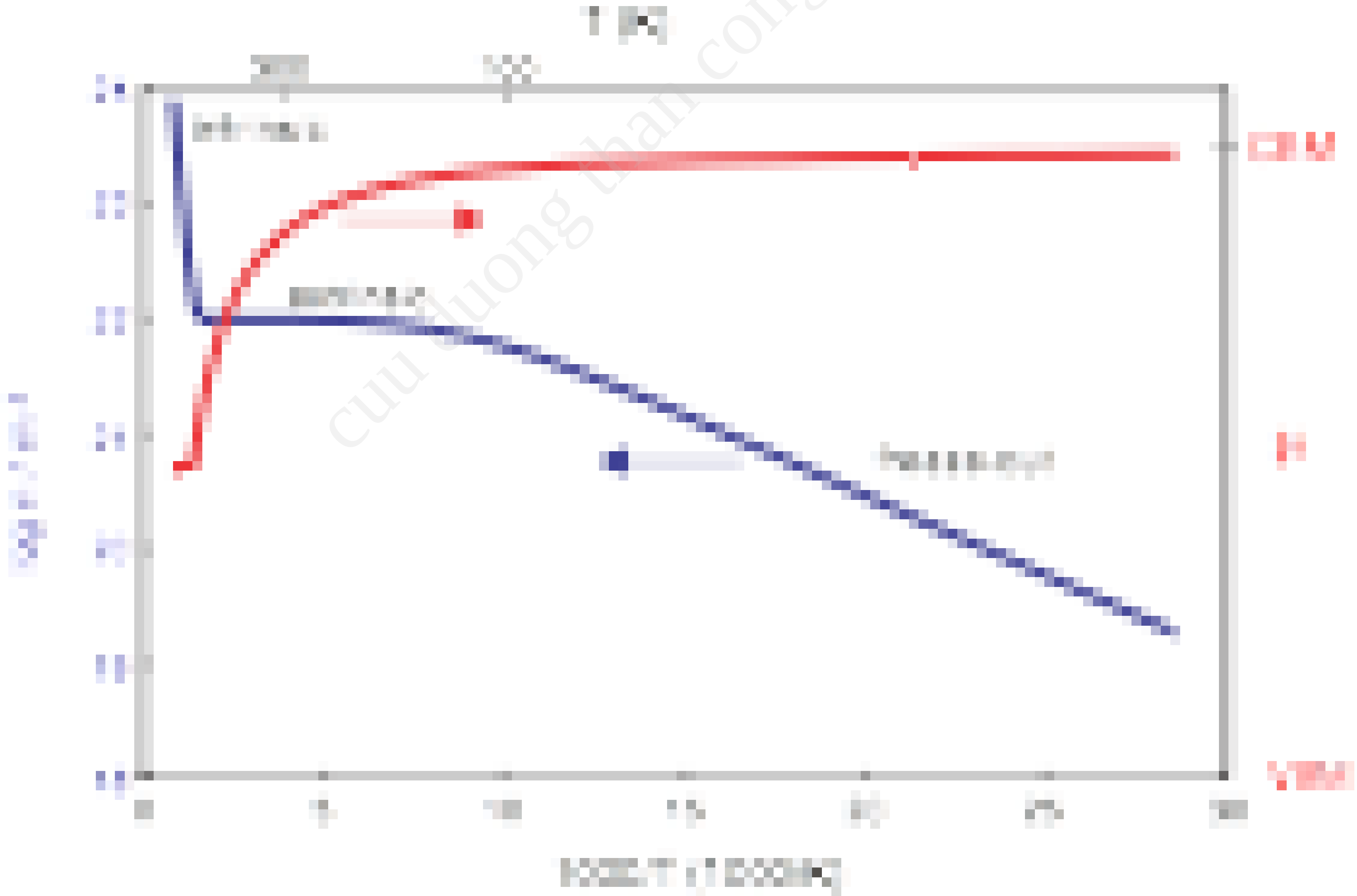

conduction band
acceptor
state
μ
E
a
E
g
valence band

Carrier concentration

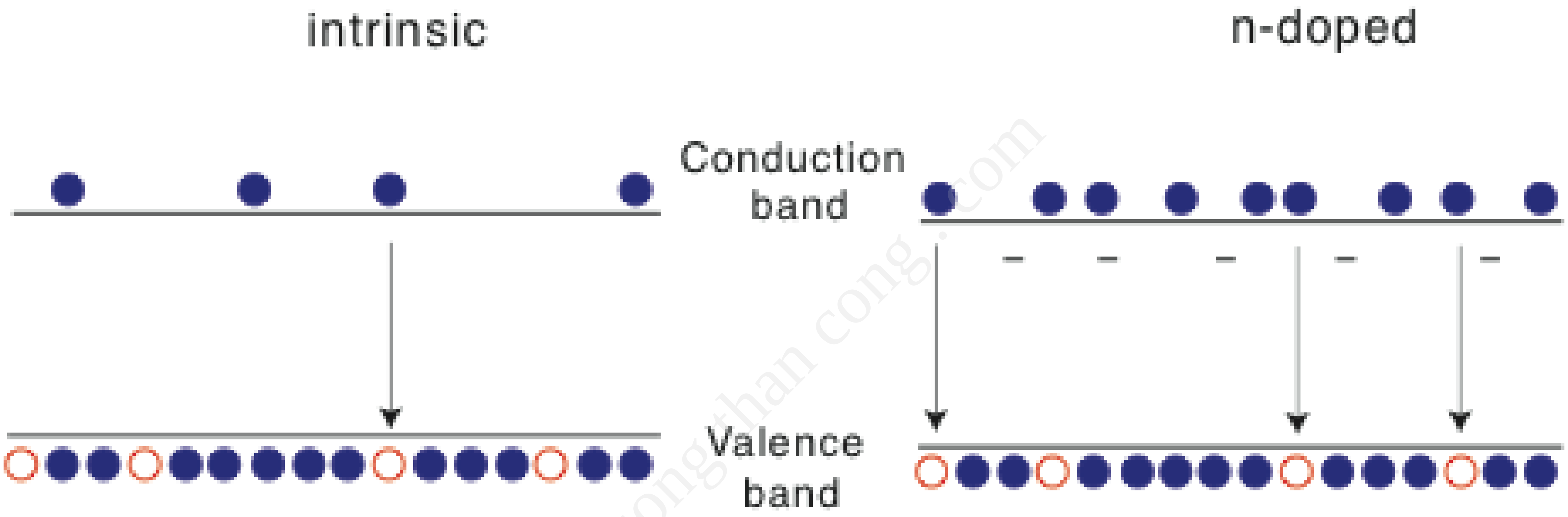
- Only numerical solution possible.
- Basis for calculation is charge neutrality.
- At very low temperature, μ must be between donor level and the conduction band minimum (n-doping).
- At very high temperature, μ must be in the middle of the gap because all donors are ionized.




High temperature (intrinsic)
Intermediate temperature (extrinsic)
Low temperature (freeze-out)
CB
μ
VB
CB
μ
VB


T [K]
200
100
intrinsic
extrinsic
freeze-out
CBM
μ
VBM
0
5
10
15
20
25
30
1000/T [1000/K]

Law of mass action

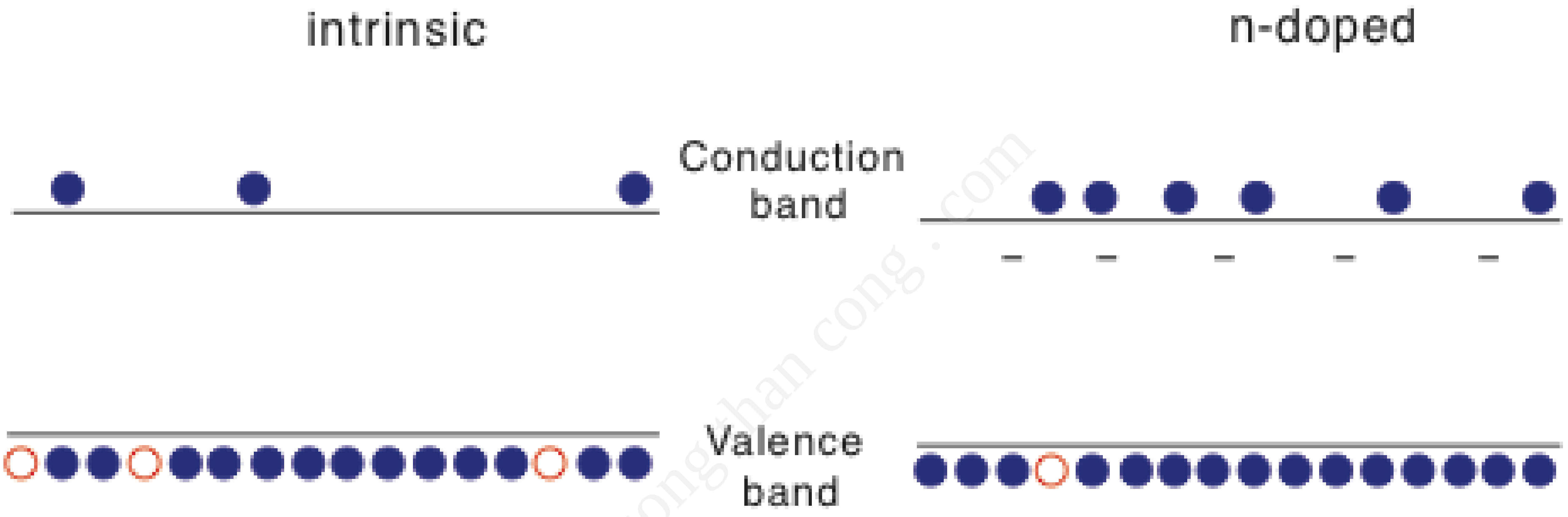


$np = n_i p_i = \text{constant}$ at a given T

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

This does not depend on the position of μ.

Majority and minority carriers

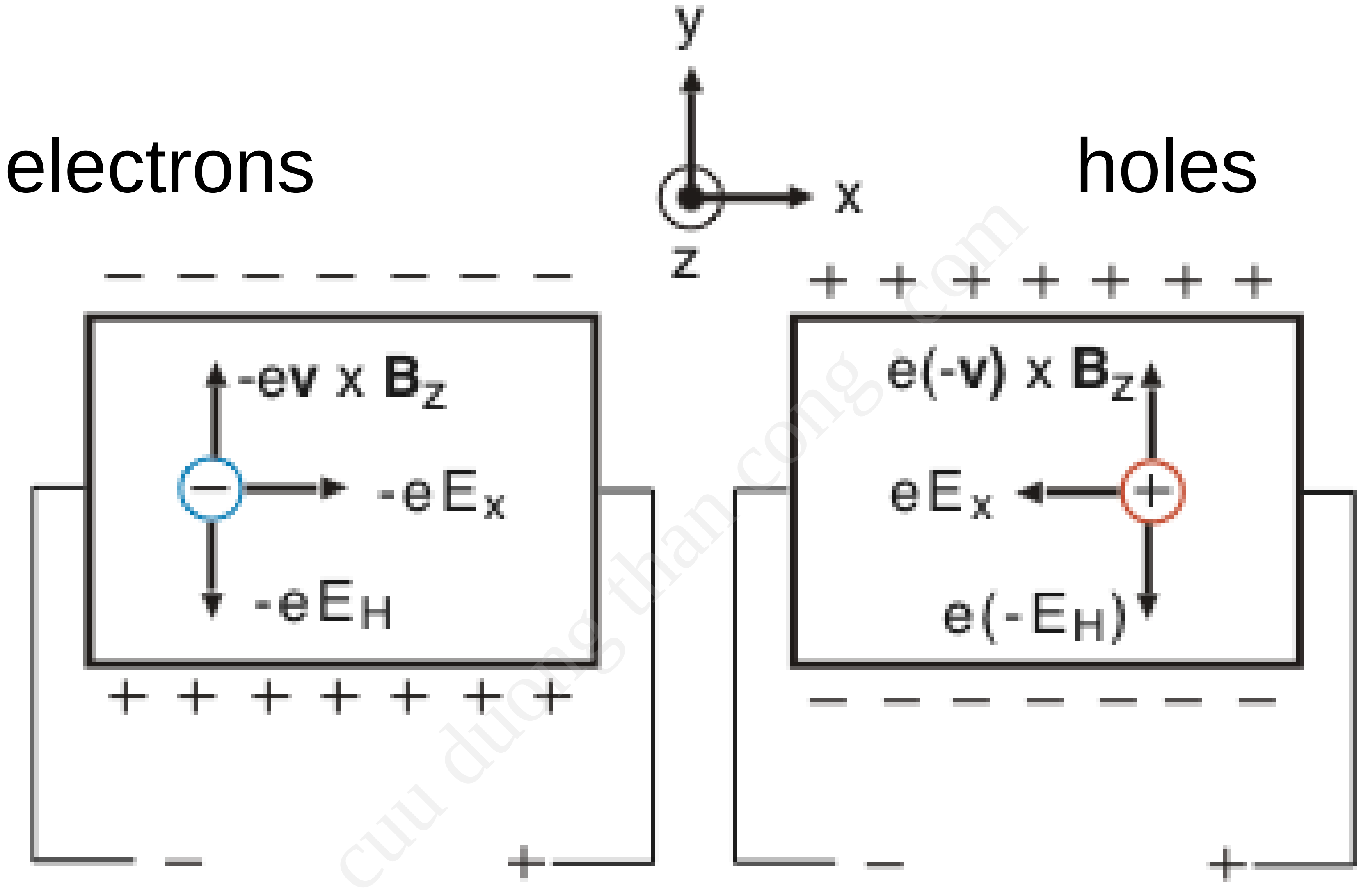


equal number of electrons and holes

majority: electrons

minority: holes

Measurement of carrier concentration: Hall effect



$$R_H = \frac{-1}{ne}$$

$$R_H = \frac{1}{pe}$$

The total conductivity

just for electrons: conductivity

$$\sigma = \frac{ne^2\tau}{m_e^*} = n\mu e$$

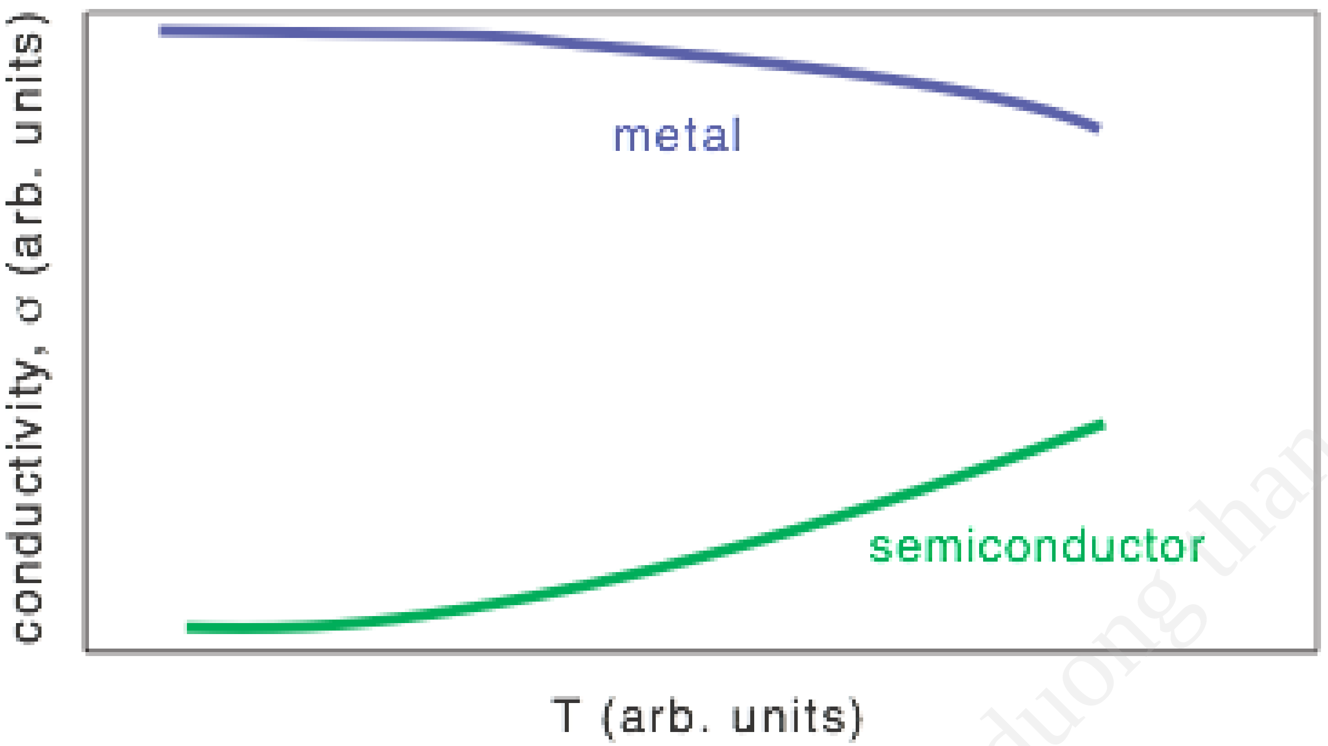
mobility $$\mu = \frac{e\tau}{m_e^*}$$

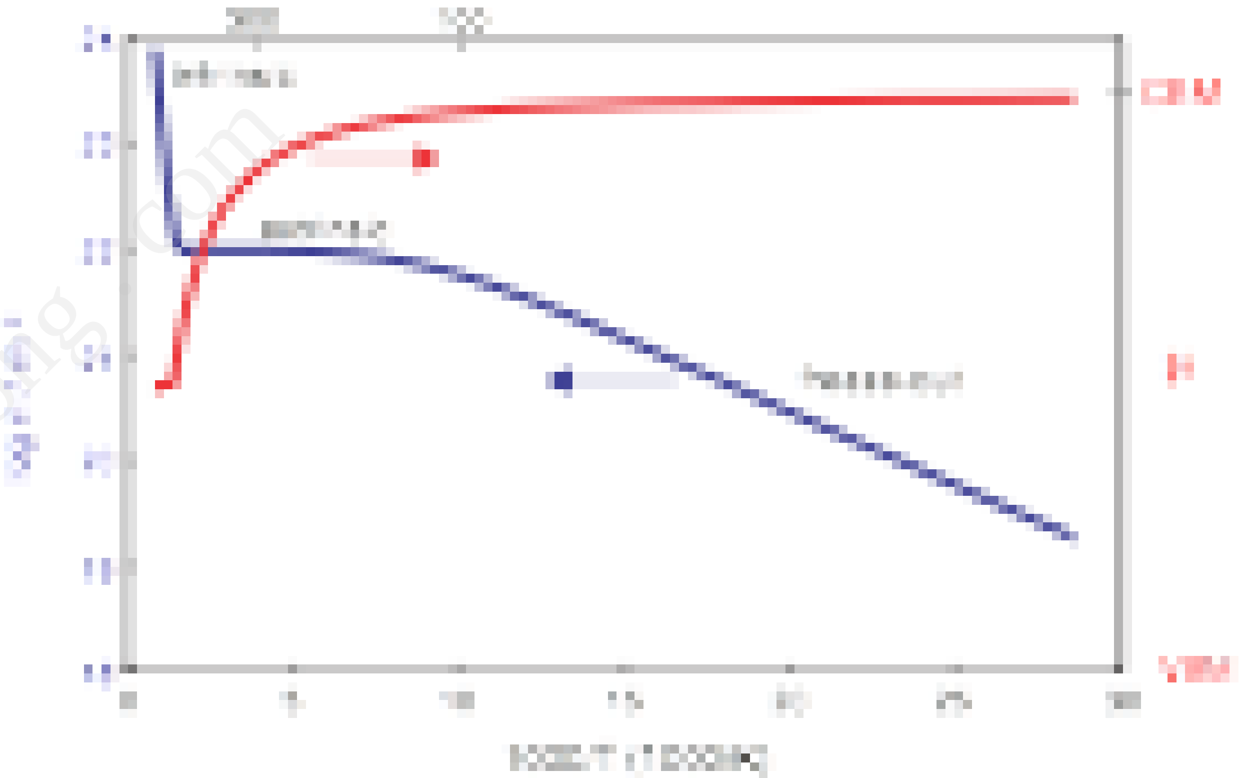
concentrations

$$\sigma = |e|(n\mu_e + p\mu_h)$$

mobilities

Temperature-dependent conductivity

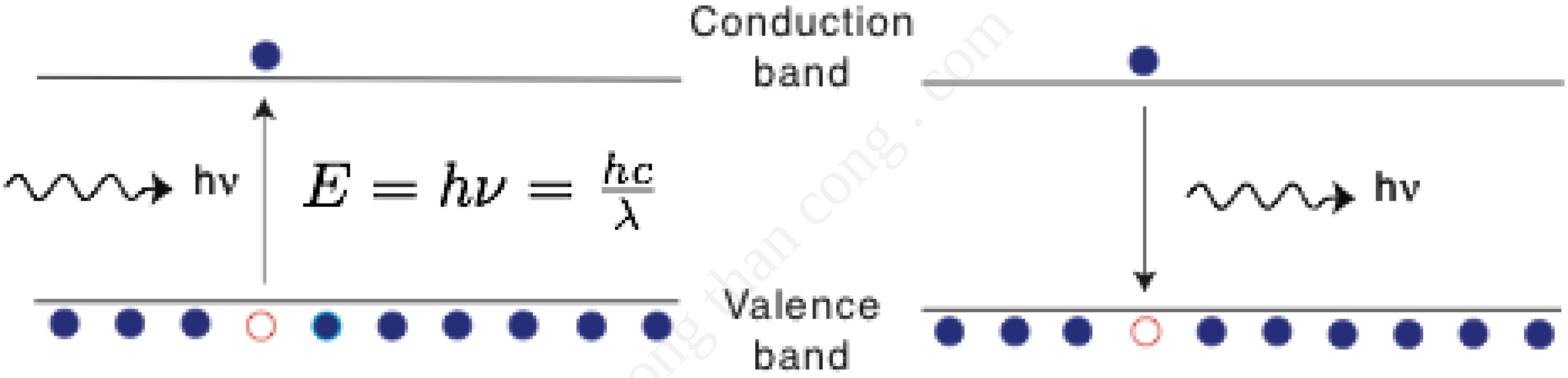




$$\sigma = \frac{ne^2\tau}{m_e} = n\mu e$$

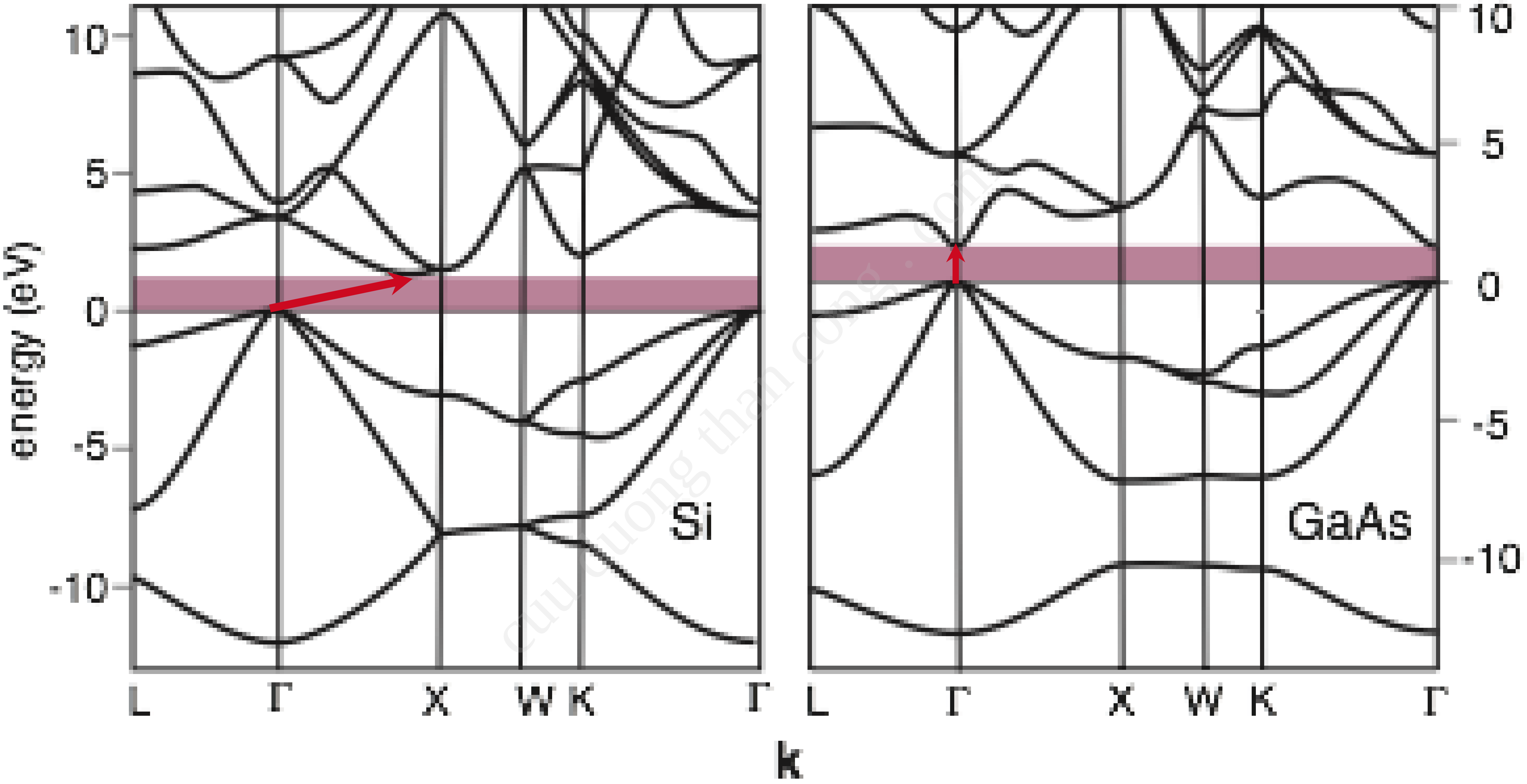
Optical properties

light absorption   light emission



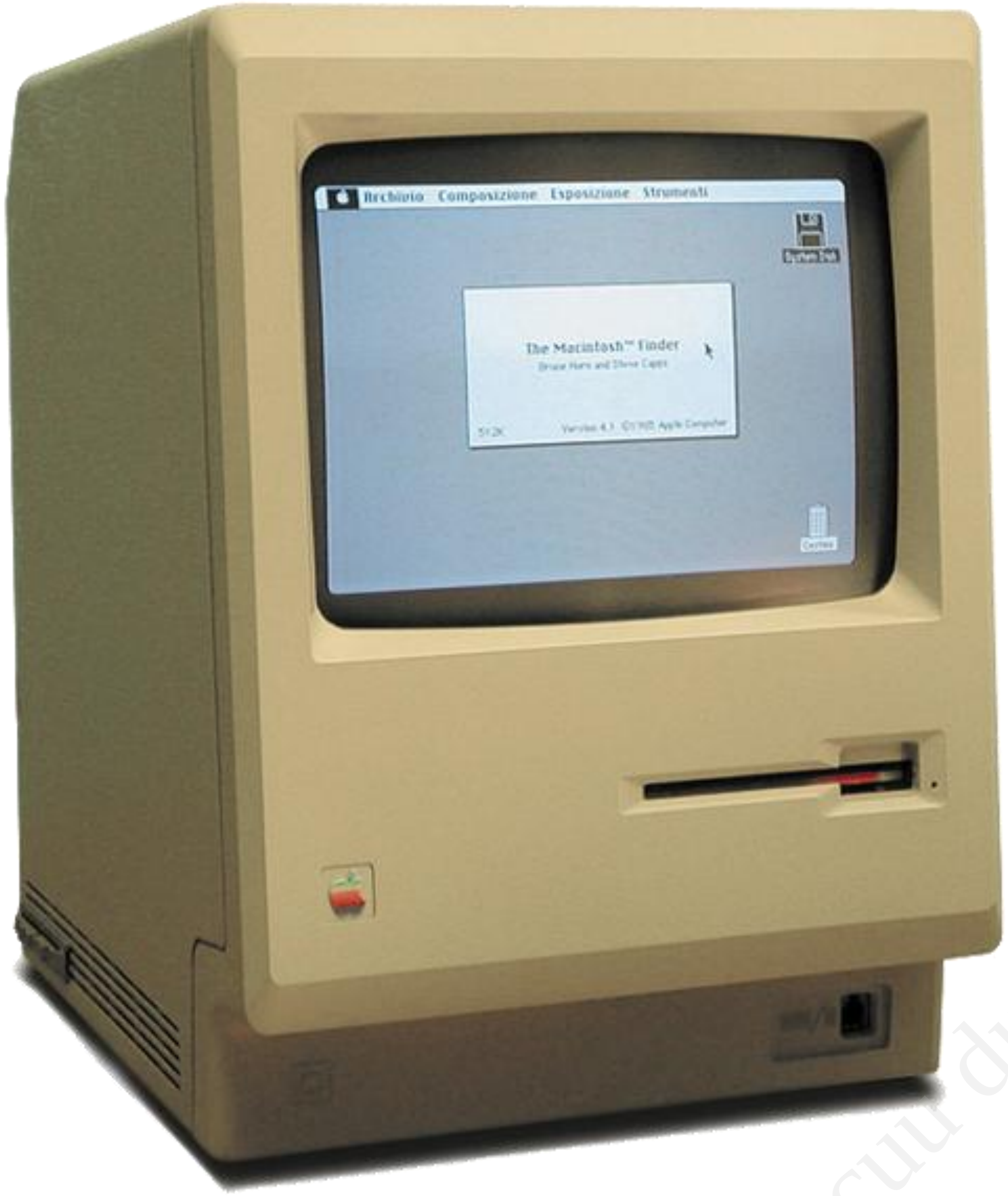
visible spectrum: 1.7 to 3.1 eV

Optical properties



- Optical photons carry energy but almost no momentum.
- A transition with a change in k can therefore not be achieved.

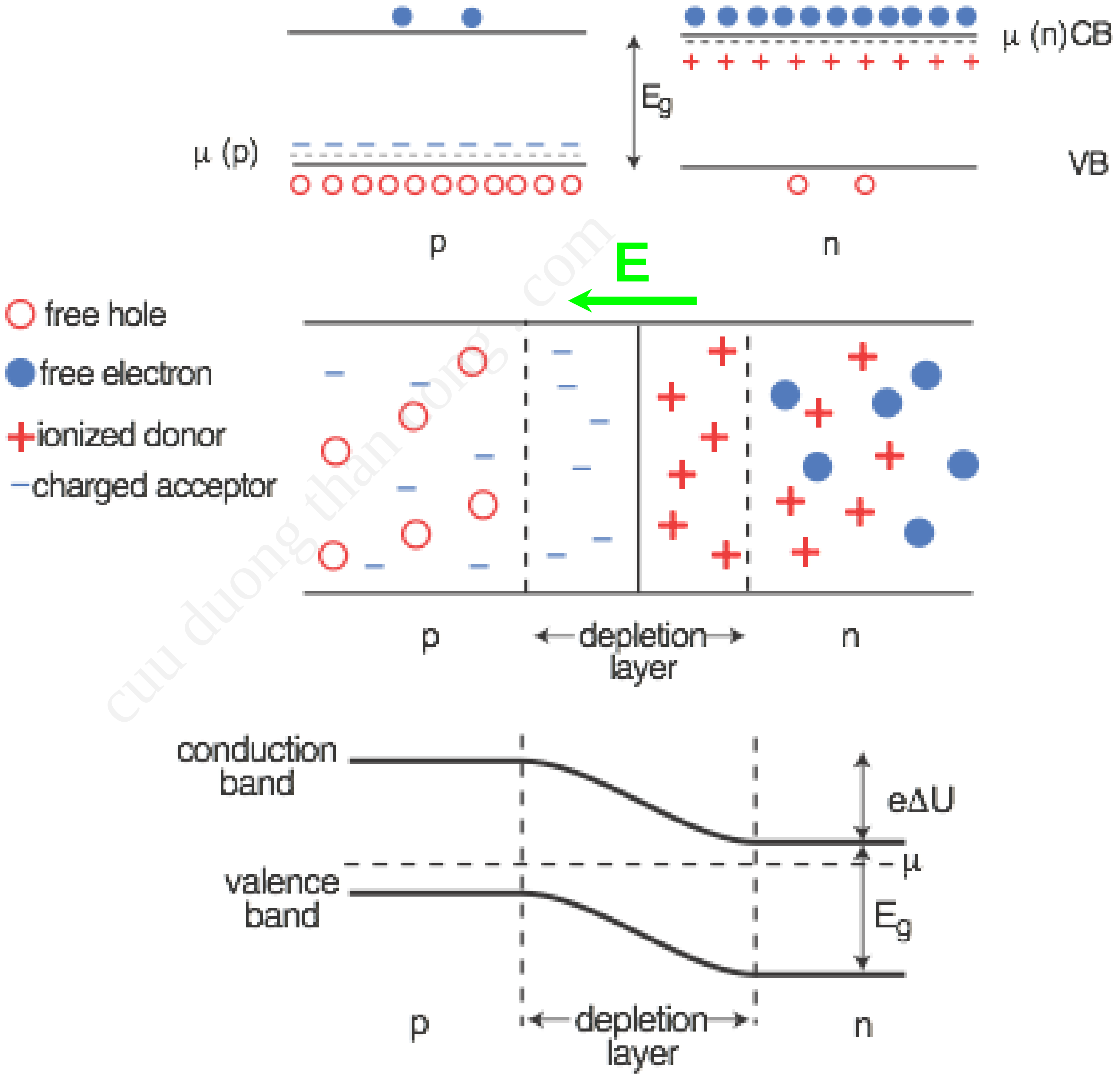
Semiconductor devices

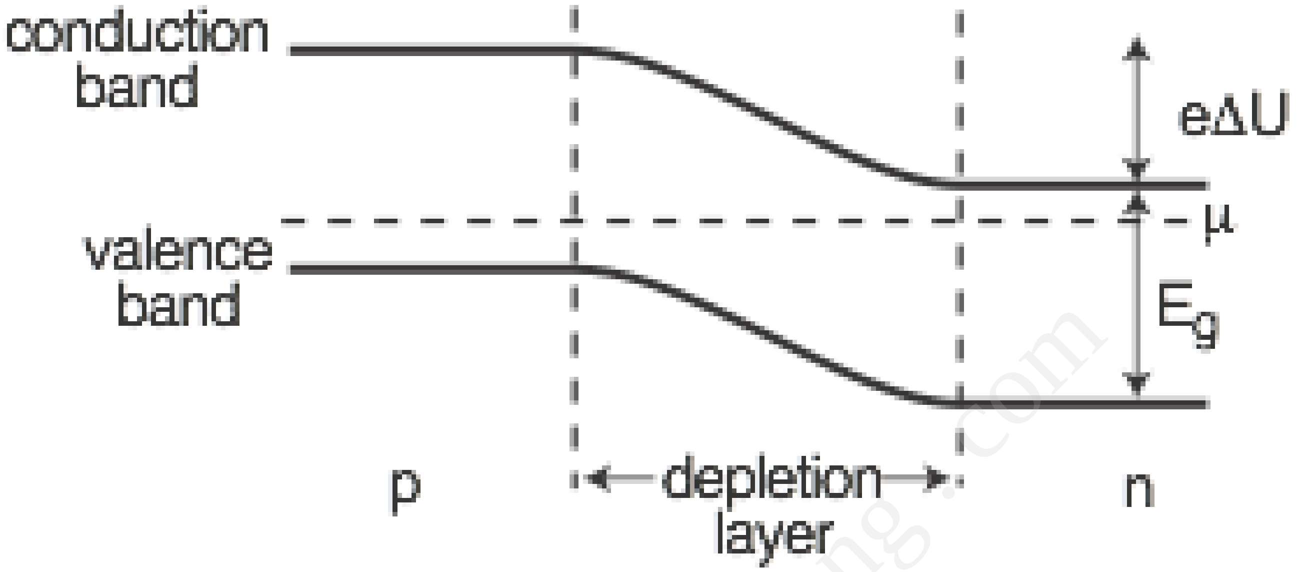


- The conductivity can be controlled by an electric field.
- Turn electricity into light and vice versa.

The p-n junction

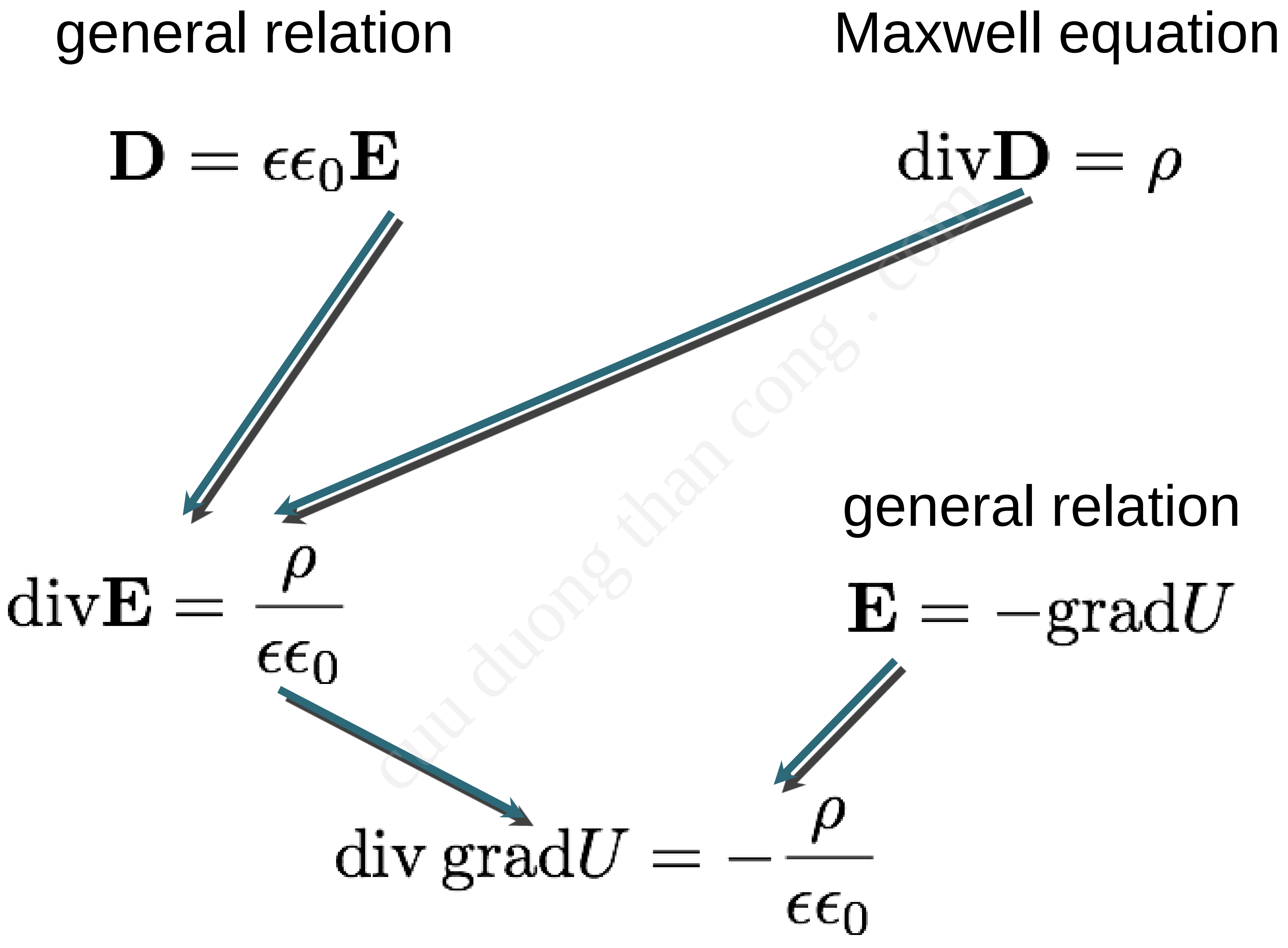
(of identical semiconductor material)





- What is the potential difference?
- What is the length of the depletion zones?

Origin of Poisson’s equation



general relation

$$\mathbf{D} = \epsilon\epsilon_0\mathbf{E}$$

Maxwell equation

$$\mathrm{div}\mathbf{D} = \rho$$

$$\mathrm{div}\mathbf{E} = \frac{\rho}{\epsilon\epsilon_0}$$

general relation

$$\mathbf{E} = -\mathrm{grad}U$$

$$\mathrm{div}\,\mathrm{grad}U = -\frac{\rho}{\epsilon\epsilon_0}$$

$$\frac{d^2U}{dx^2} = -\frac{\rho}{\varepsilon\varepsilon_0}$$

The p-n junction: quantitative solution

assume: no free carriers in depletion region

$$\rho_p = -eN_a$$

and

$$\rho_n = +eN_d$$

$$N_a d_p = N_d d_n$$

Poisson's equation

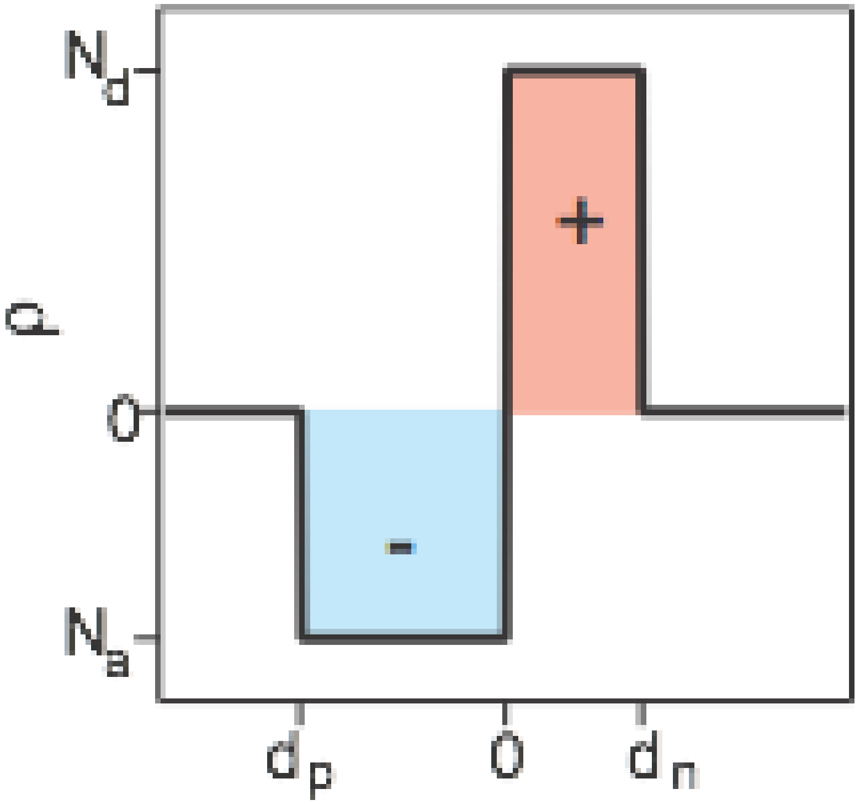
$$\frac{d^2U}{dx^2} = -\frac{\rho}{\epsilon\epsilon_0}$$

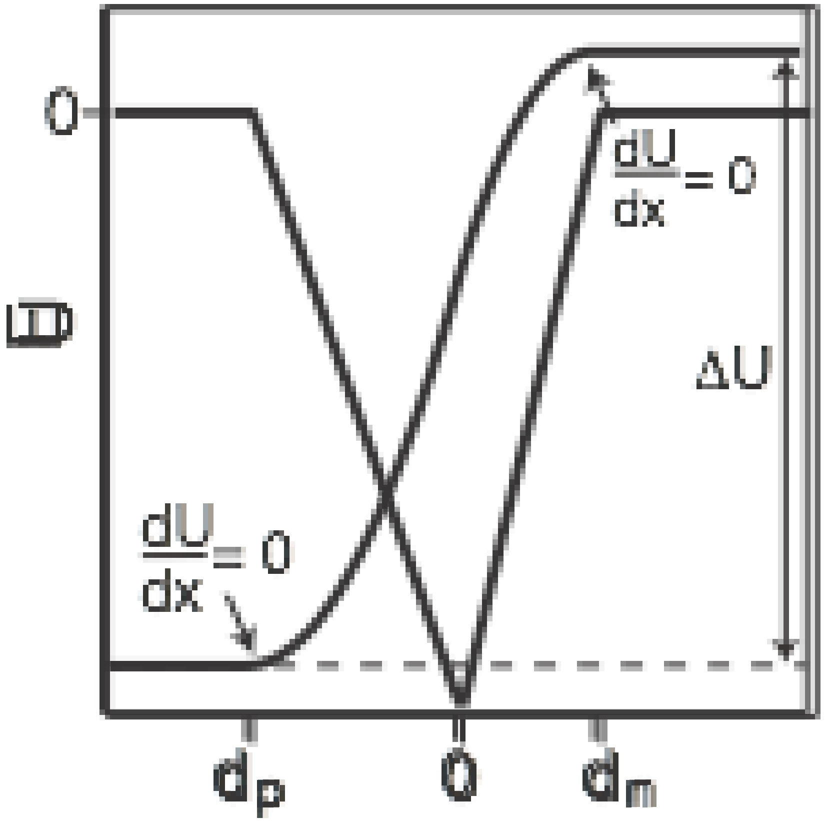
boundary conditions: U and dU/dx continuous

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

result for the total potential change

$$\Delta U = \frac{e}{2\epsilon\epsilon_0}\left(N_d d_n^2 + N_a d_p^2\right)$$





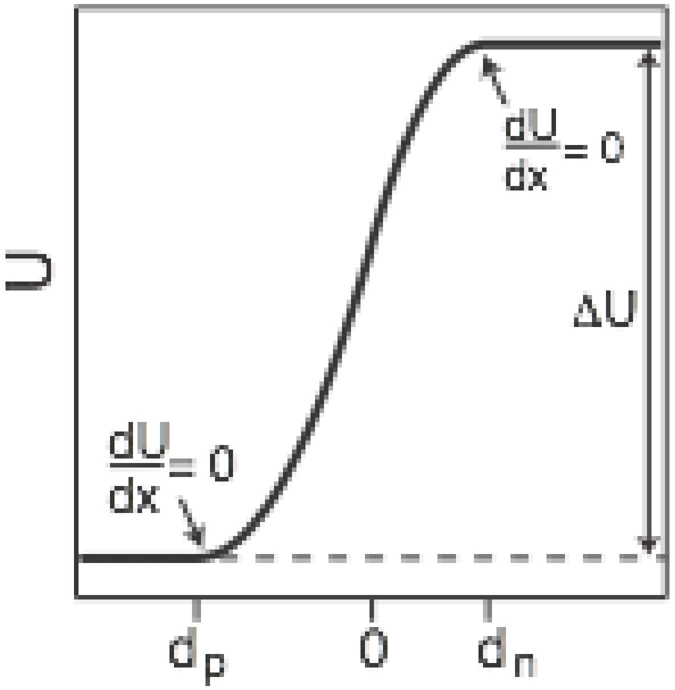
The p-n junction: quantitative solution

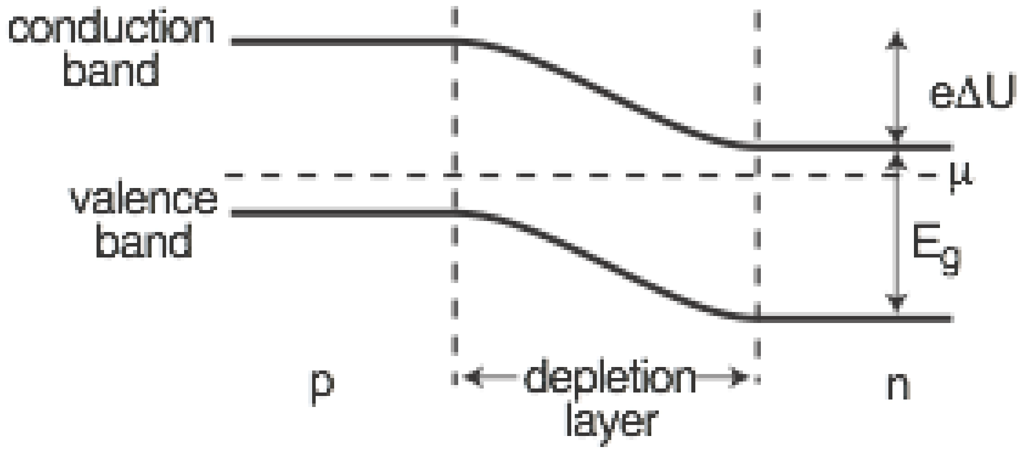
$$\Delta U = \frac{e}{2\epsilon\epsilon_0}\left(N_d d_n^2 + N_a d_p^2\right) \longleftarrow N_a d_p = N_d d_n$$

the length of the depletion layer

$$d_p = \left(\frac{\Delta U 2\epsilon\epsilon_0}{eN_a}\frac{N_d}{N_a + N_d}\right)^{1/2}$$

$$d_n = \left(\frac{\Delta U 2\epsilon\epsilon_0}{eN_d}\frac{N_a}{N_a + N_d}\right)^{1/2}$$





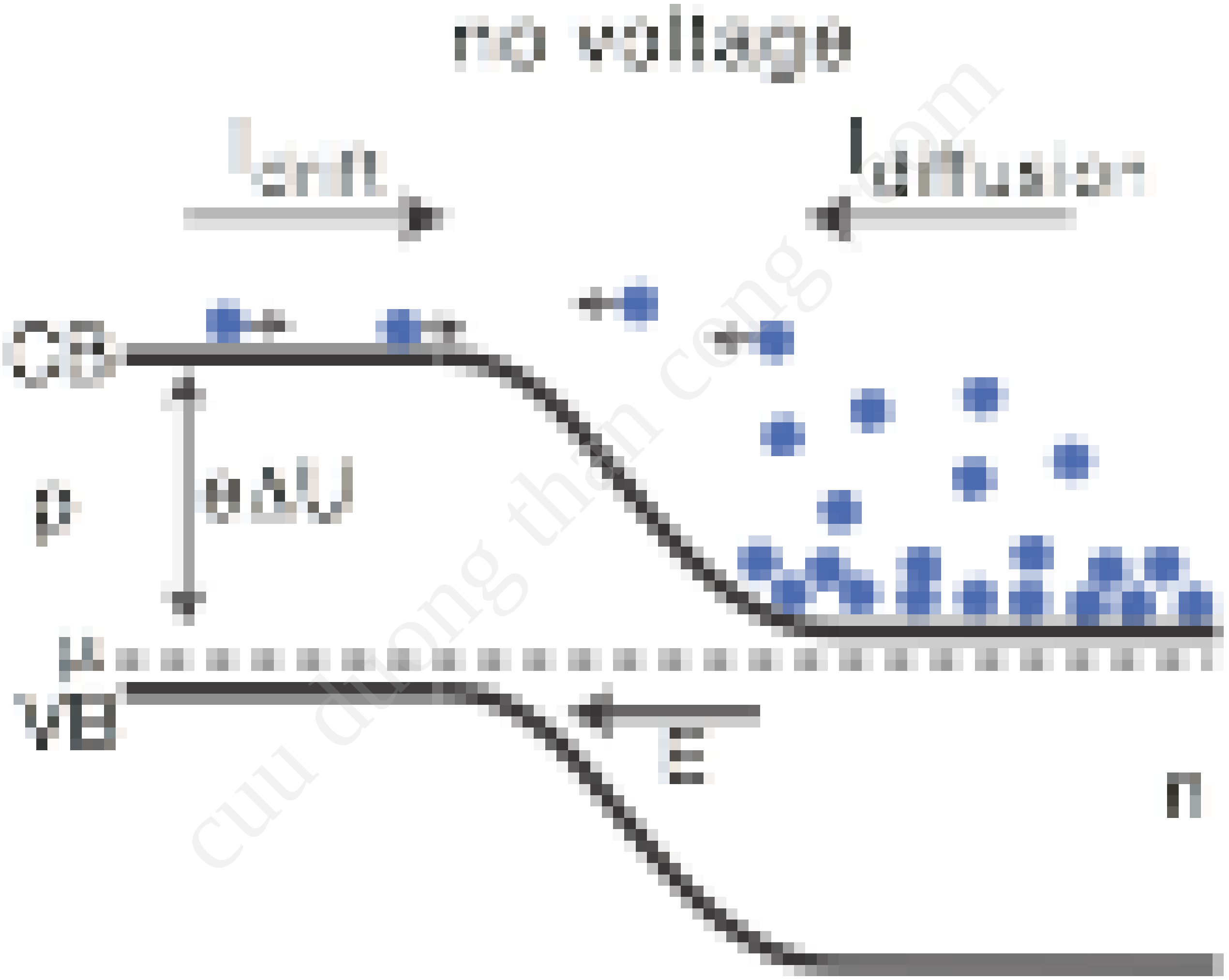
at very low T

$$\Delta U \approx E_g$$

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

The p-n junction with an applied voltage

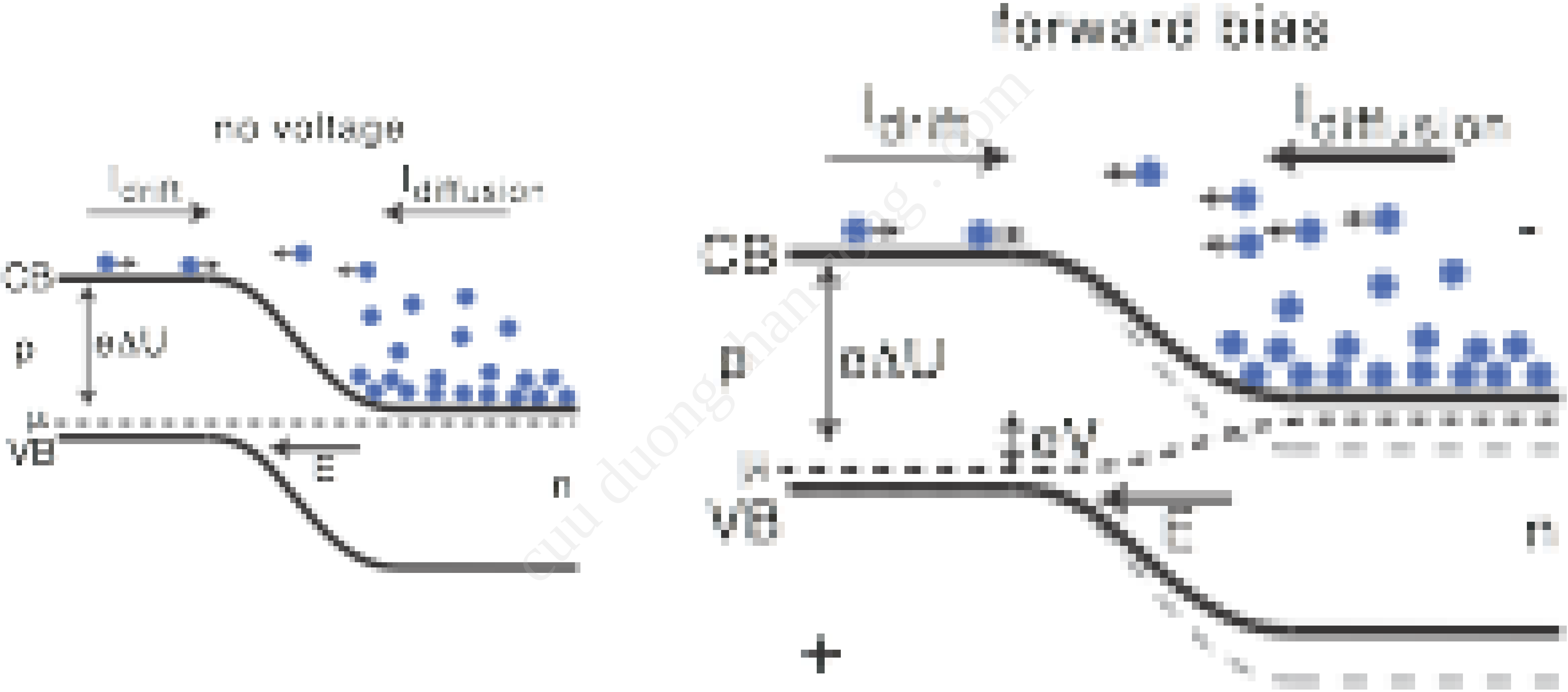
consider electrons only



- drift of minority electrons (p) and diffusing of majority electrons (n) equal.

The p-n junction with an applied voltage

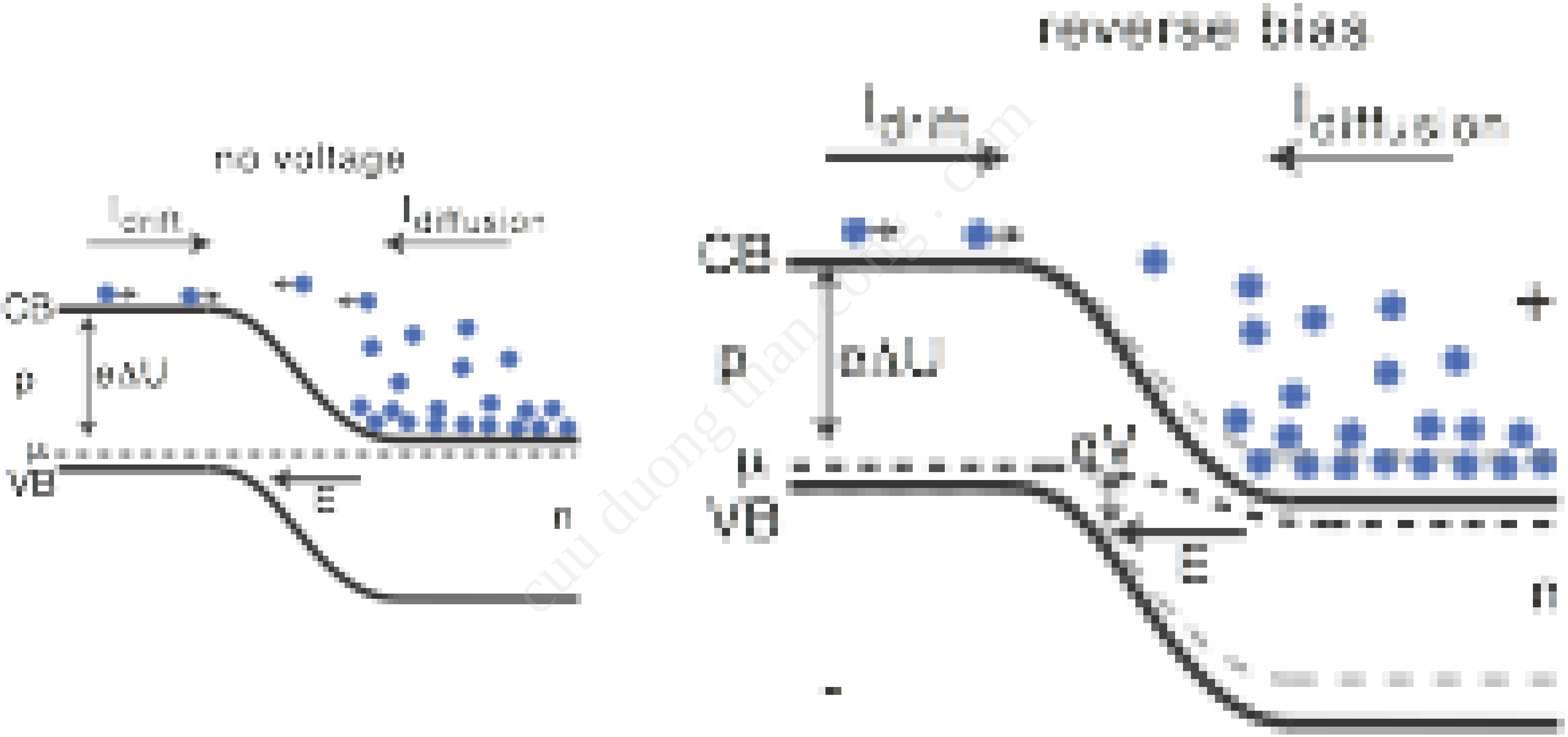
consider electrons only



- Voltage drop only over depletion zone.
- Increased diffusion current, drift current unaffected.

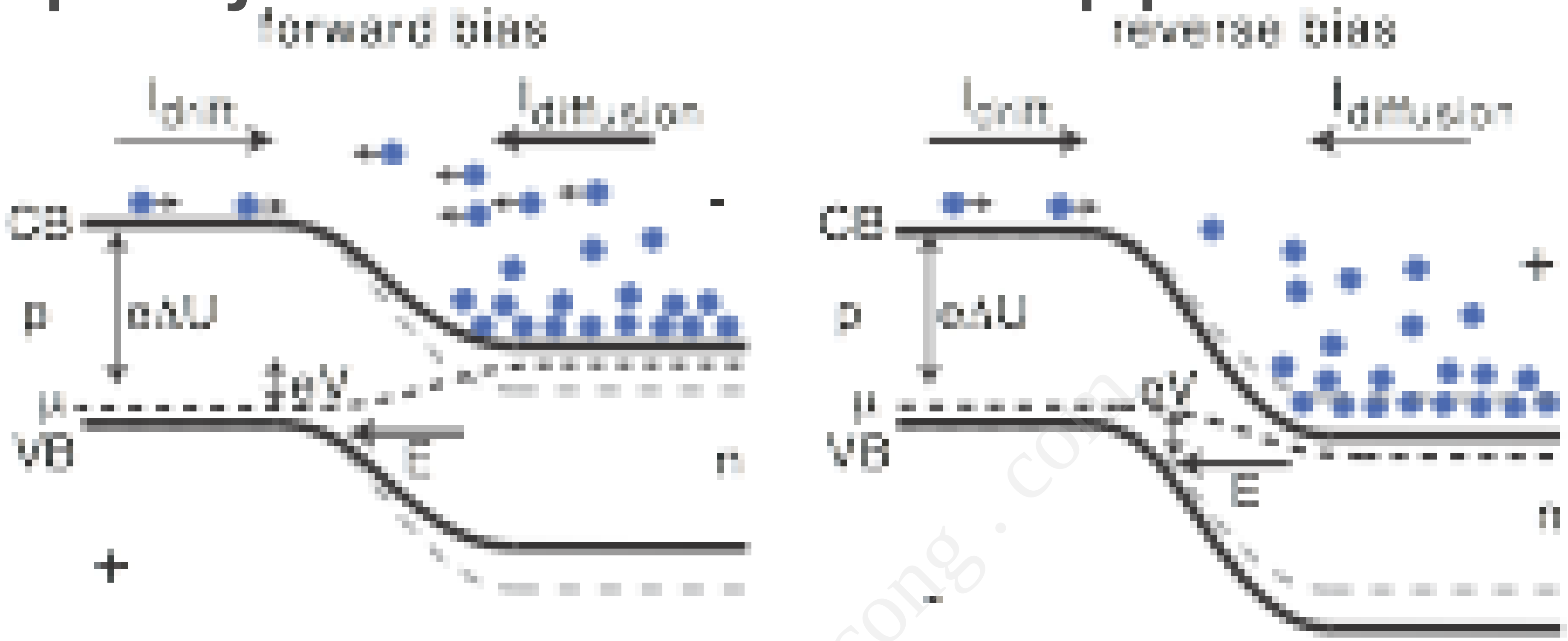
The p-n junction with an applied voltage

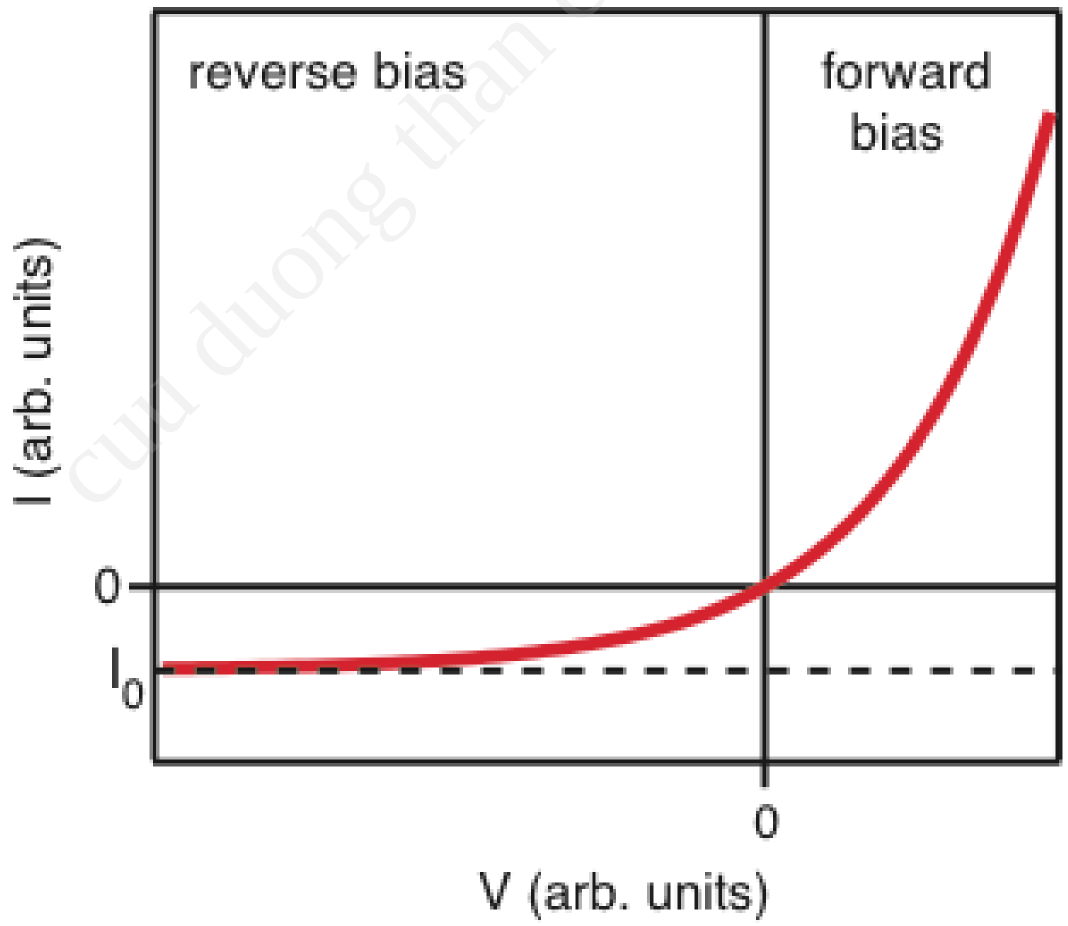
consider electrons only



- Voltage drop only over depletion zone.
- decreased diffusion current, drift current unaffected.

The p-n junction with an applied voltage

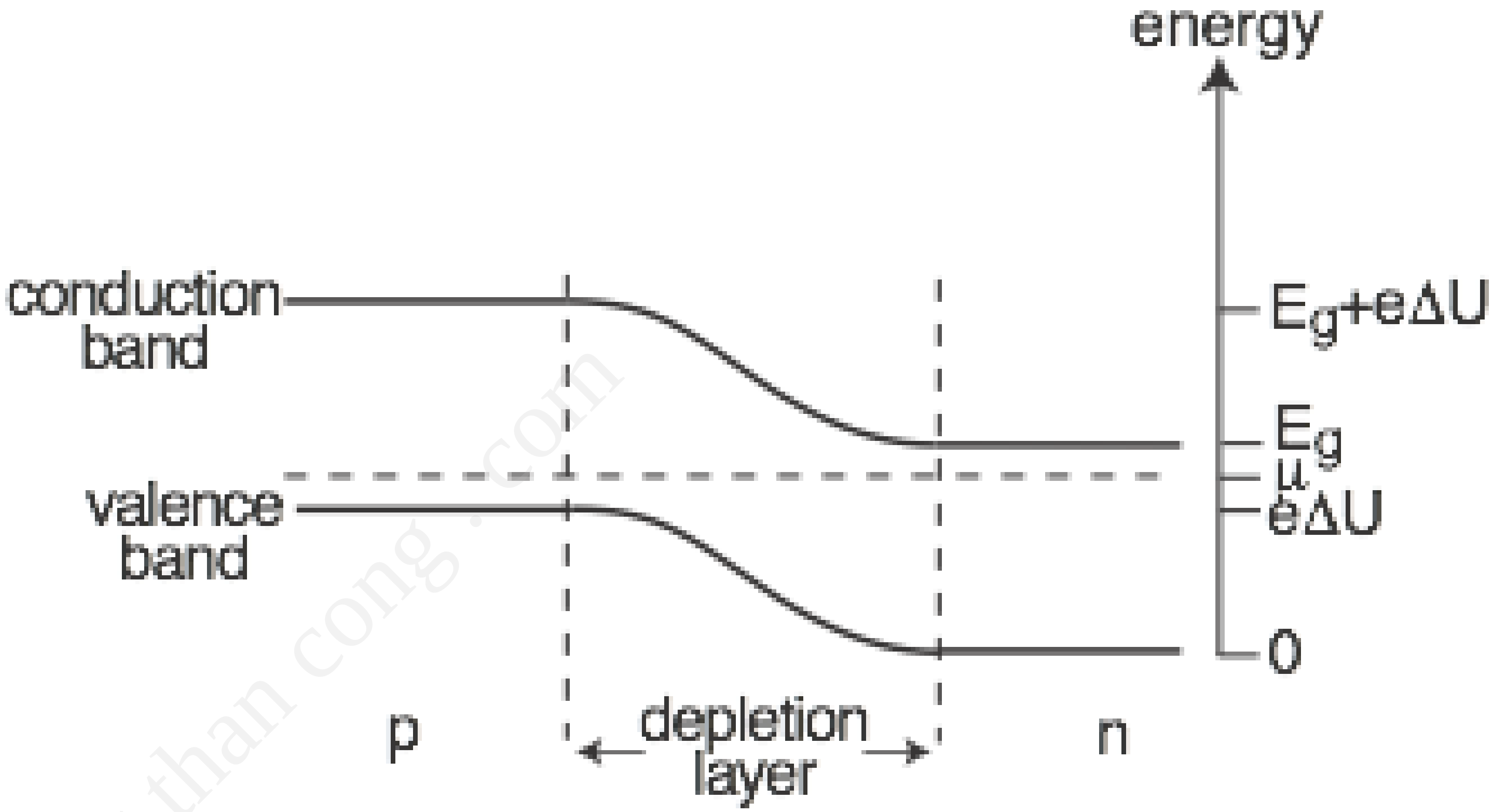




- exponential increase in forward direction
- decrease and eventual small saturation current in reverse bias

$$I = I_{\text{diffusion}} - I_{\text{drift}} = I_0\left(e^{eV/k_BT} - 1\right)$$

(very approximate) quantitative solution



calculate the carrier densities outside the depletion region

we use

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

for electrons

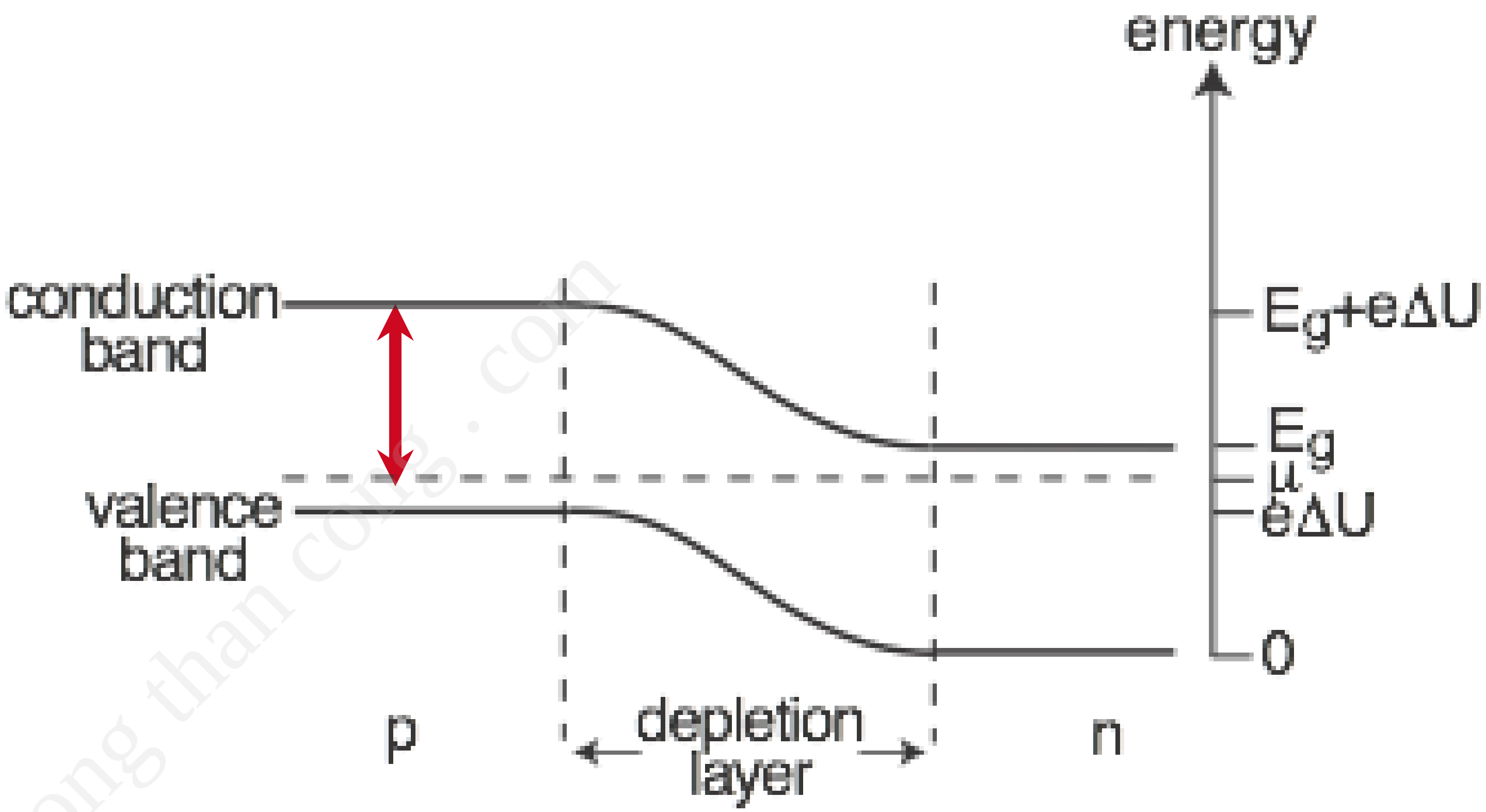
$$1 - f(E) = 1 - \frac{1}{e^{(E-\mu)/k_B T} + 1} \approx e^{(E-\mu)/k_B T}$$

for holes

(very approximate) quantitative solution

calculate the carrier densities outside the depletion region.

The VB maximum of the n-side is the energy zero.



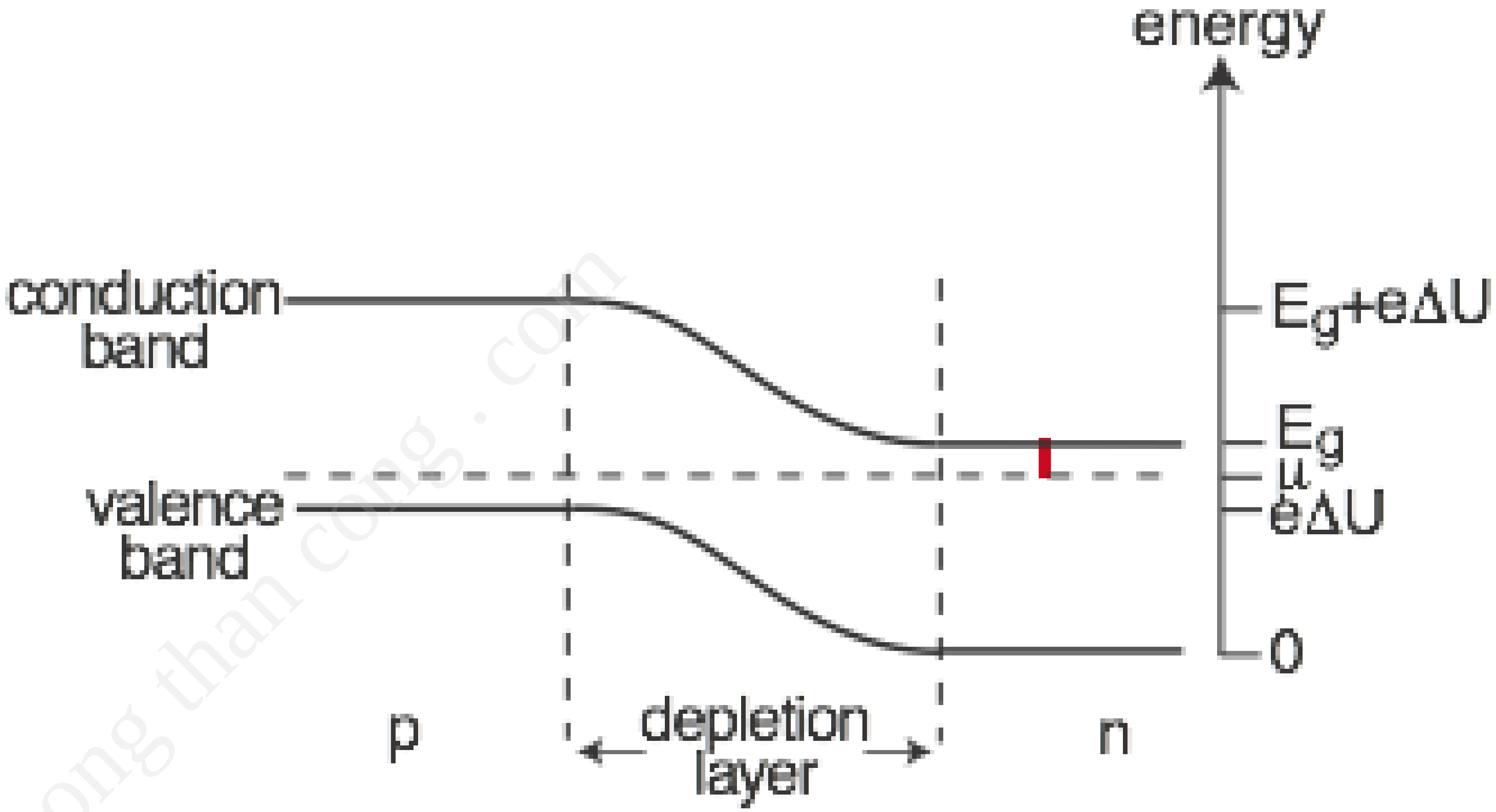
we use

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

$$n_p = N_c e^{(\mu-E_g-e\Delta U)/k_BT}$$

(very approximate) quantitative solution

calculate the carrier densities outside the depletion region



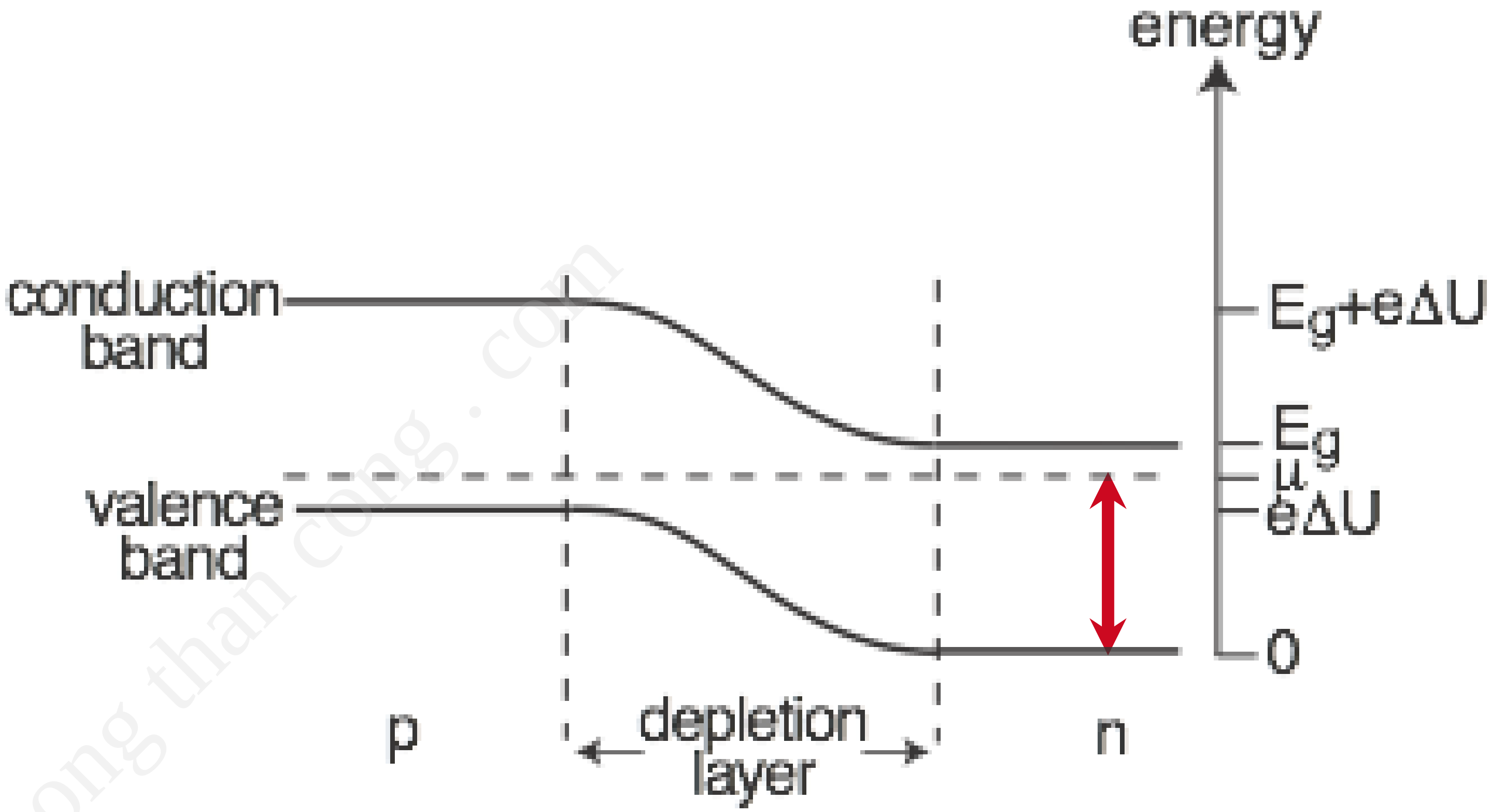
we use

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

$$n_n = N_c e^{(\mu-E_g)/k_BT}$$

(very approximate) quantitative solution

calculate the carrier densities
outside the depletion region



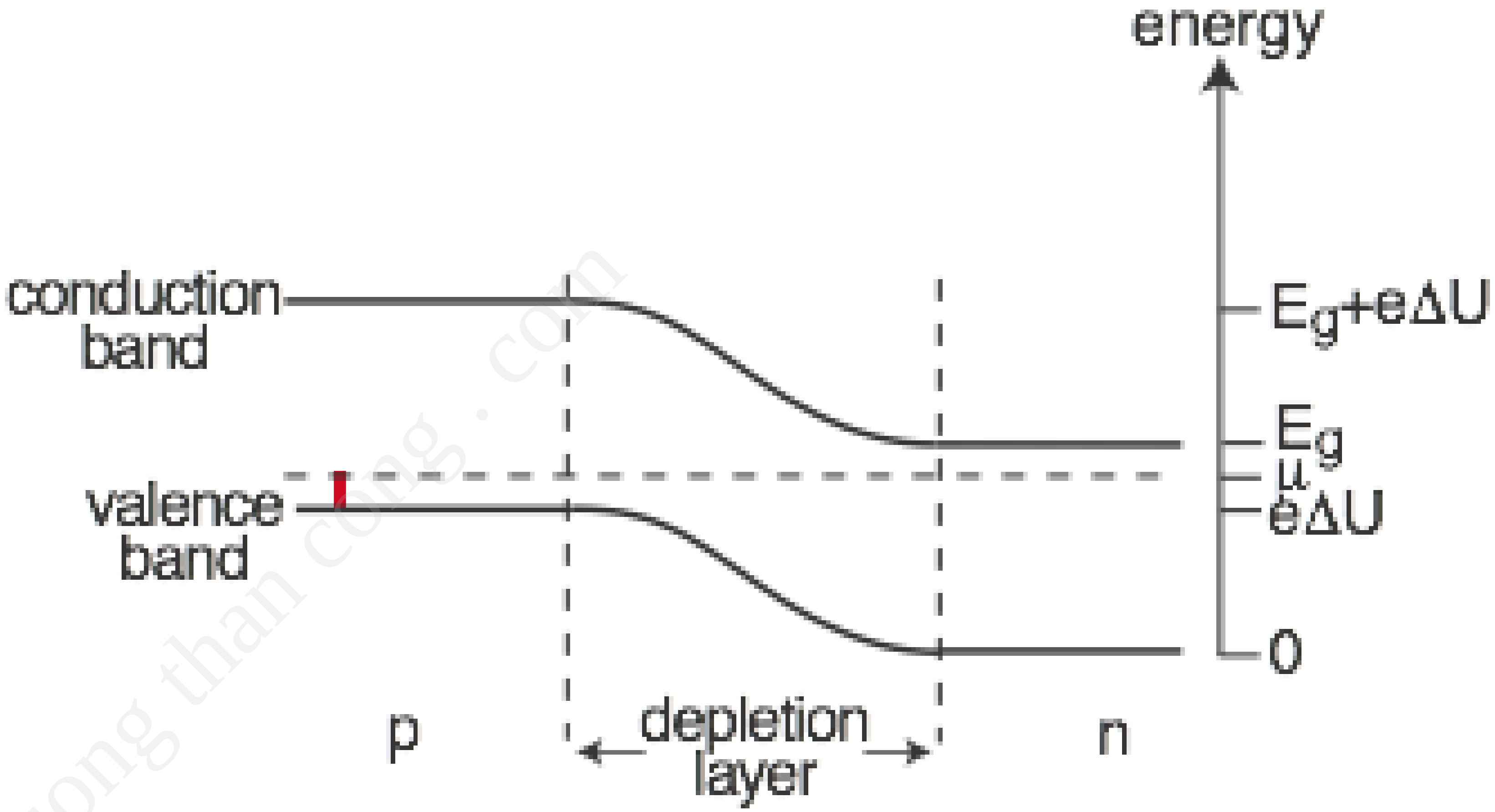
we use

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

$$p_n = N_v e^{-\mu/k_BT}$$

(very approximate) quantitative solution

calculate the carrier densities outside the depletion region

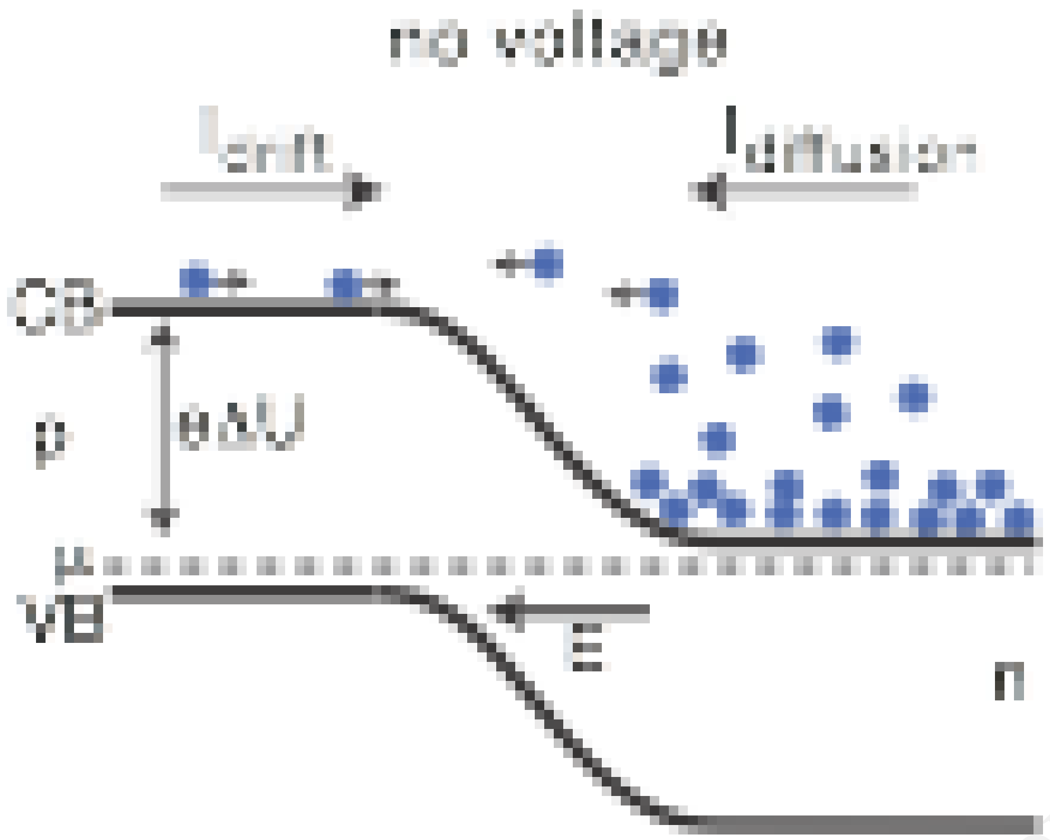


we use

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

$$p_p = N_v e^{(e\Delta U - \mu)/k_BT}$$

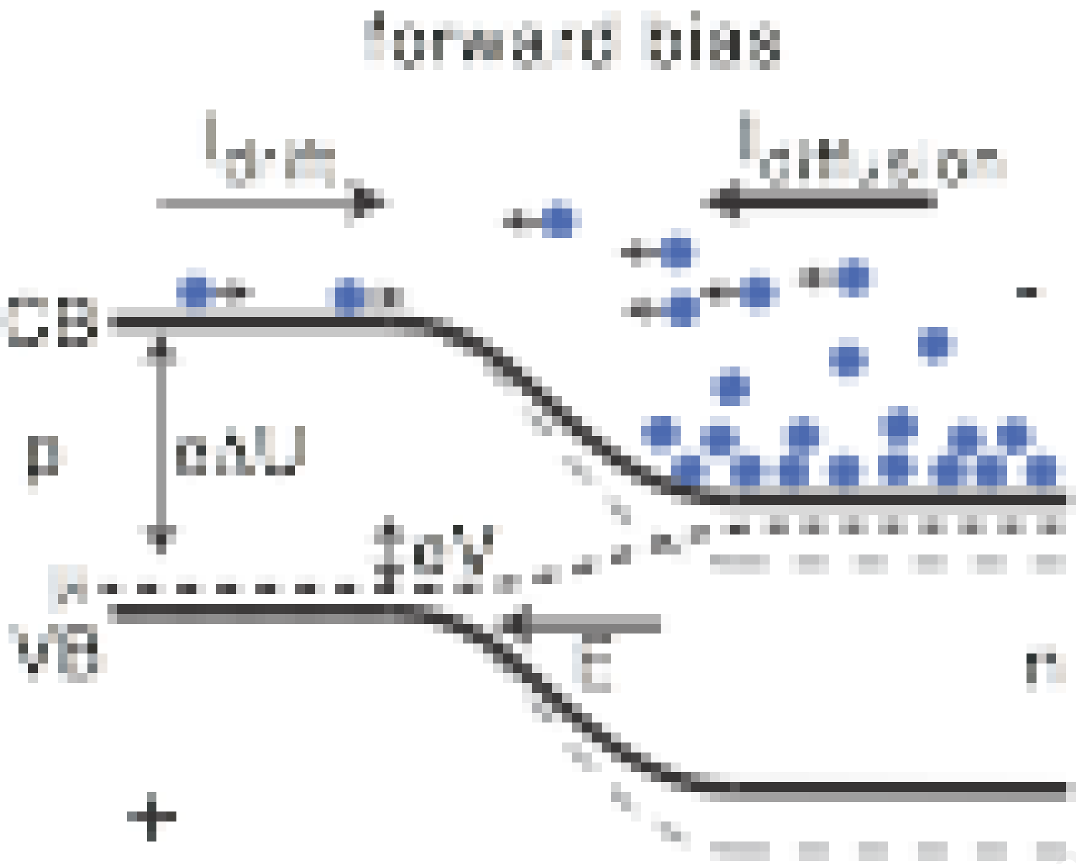
The p-n junction with an applied voltage

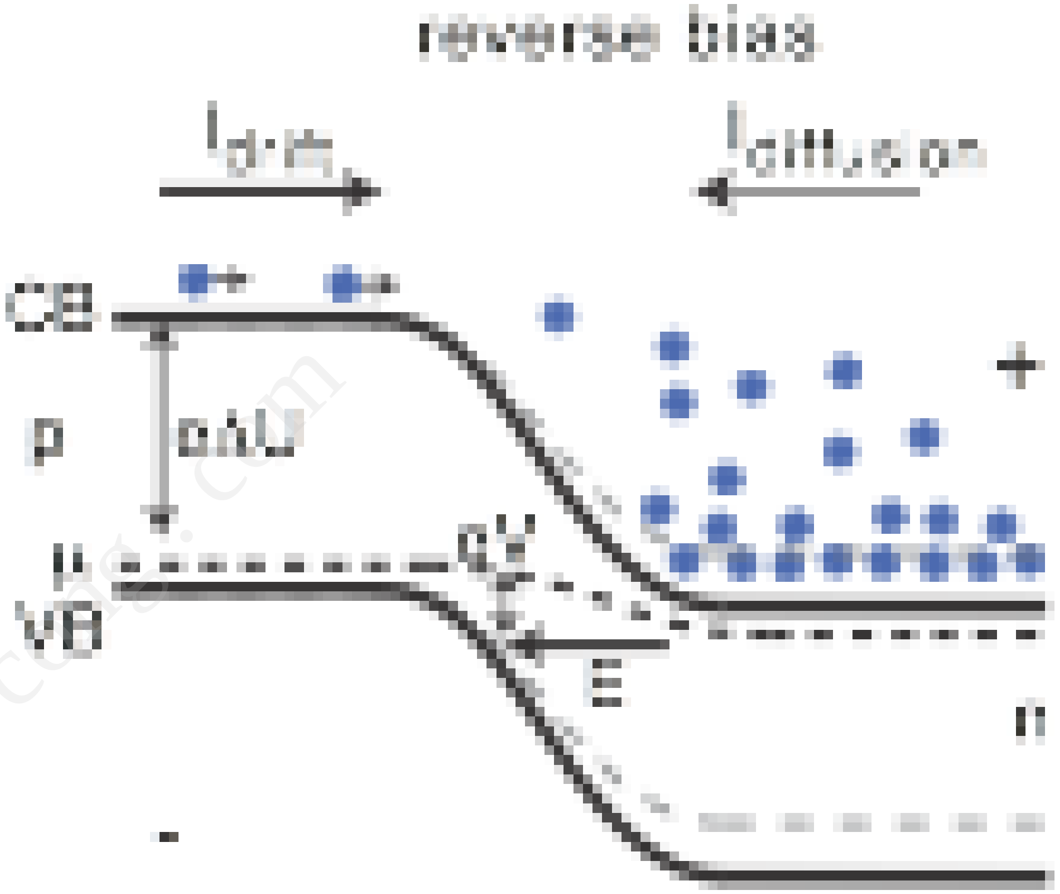


first consider no bias voltage

$$|I_{\text{diffusion}}| = |I_{\text{drift}}| = |I_0| = Ce^{(\mu - E_g - e\Delta U)/k_B T}$$

The p-n junction with an applied voltage



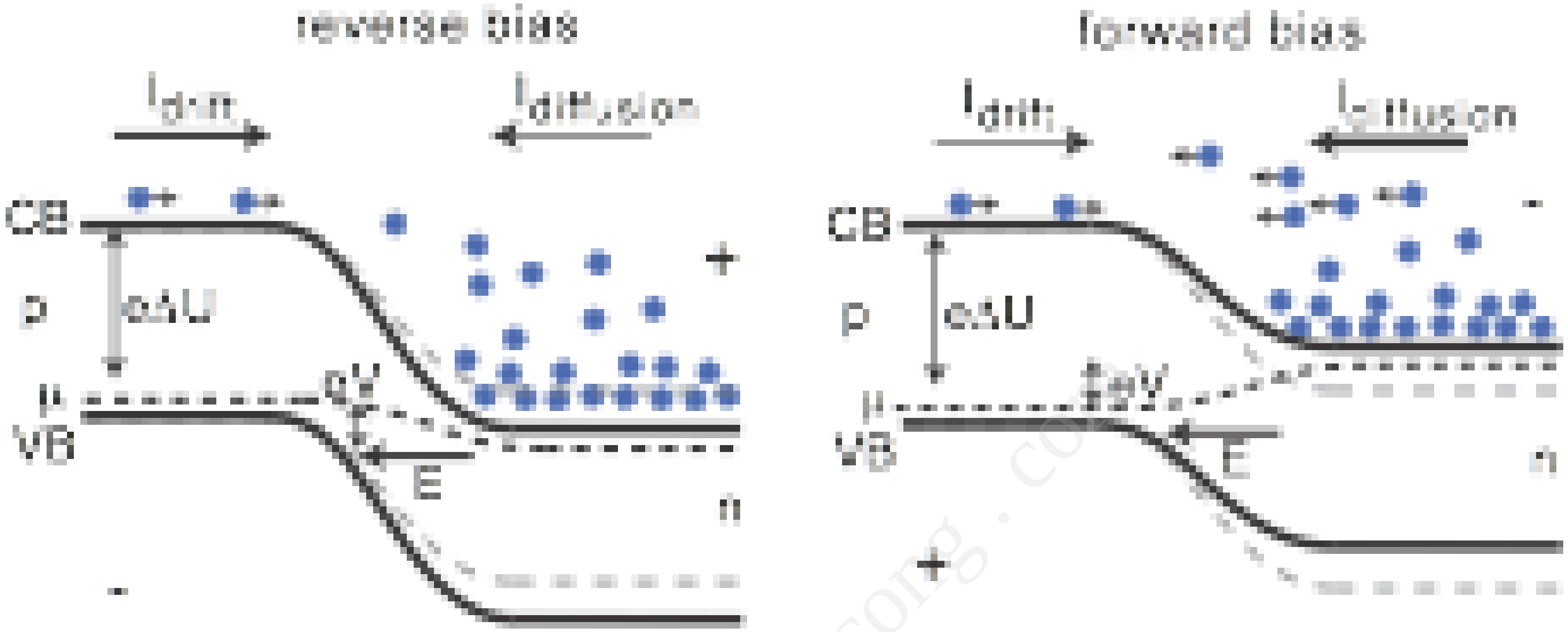


$$|I_{\text{drift}}| = |I_0| = Ce^{(\mu - E_g - e\Delta U)/k_B T};$$

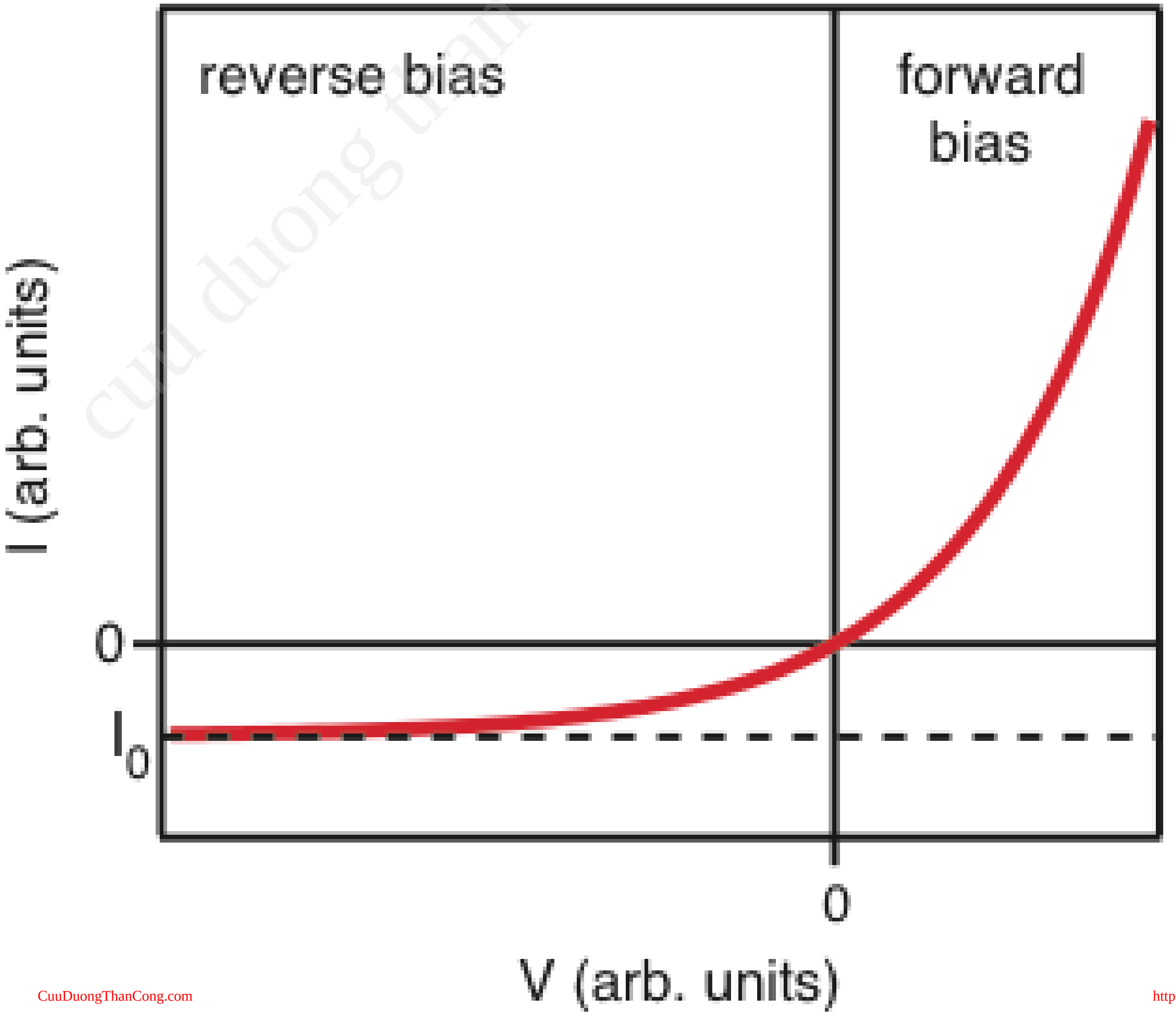
$$|I_{\text{diffusion}}| = Ce^{((\mu + eV) - E_g - e\Delta U)/k_B T}.$$

$$I = I_{\text{diffusion}} - I_{\text{drift}} = I_0\left(e^{eV/k_B T} - 1\right)$$

The p-n junction with an applied voltage



- exponential increase in forward direction
- decrease and eventual small saturation current in reverse bias

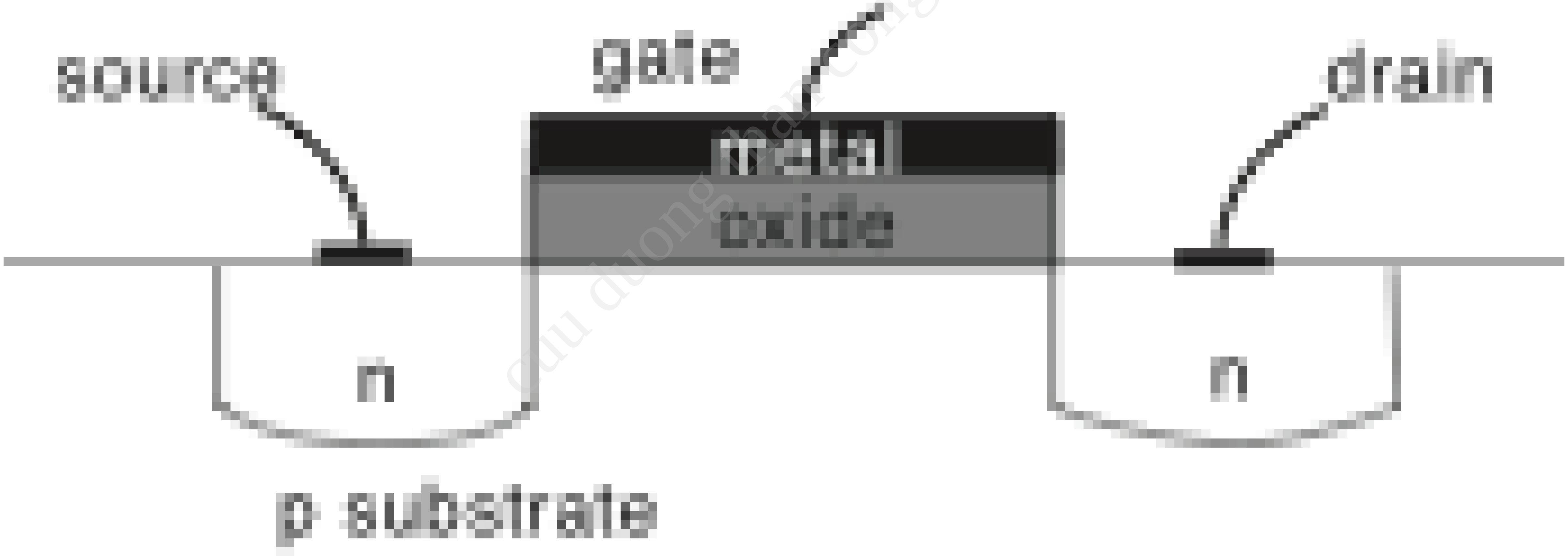


- For the holes, we can construct exactly the same arguments.

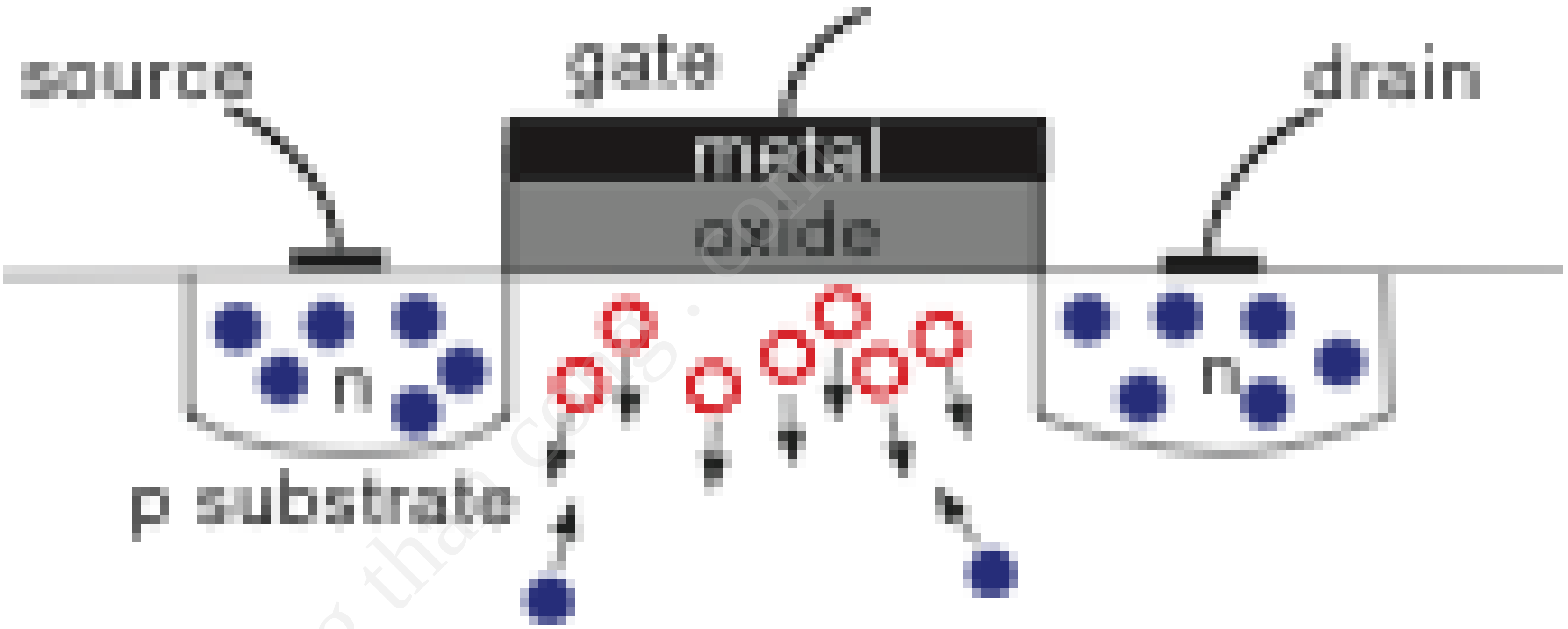
Transistors

- Two types: bipolar transistors and field-effect transistors.
- Bipolar transistors can be found as separate devices and in integrated circuits.
- Field-effect transistors can only be found in integrated circuits.
- Both can be used as amplifiers and switches.

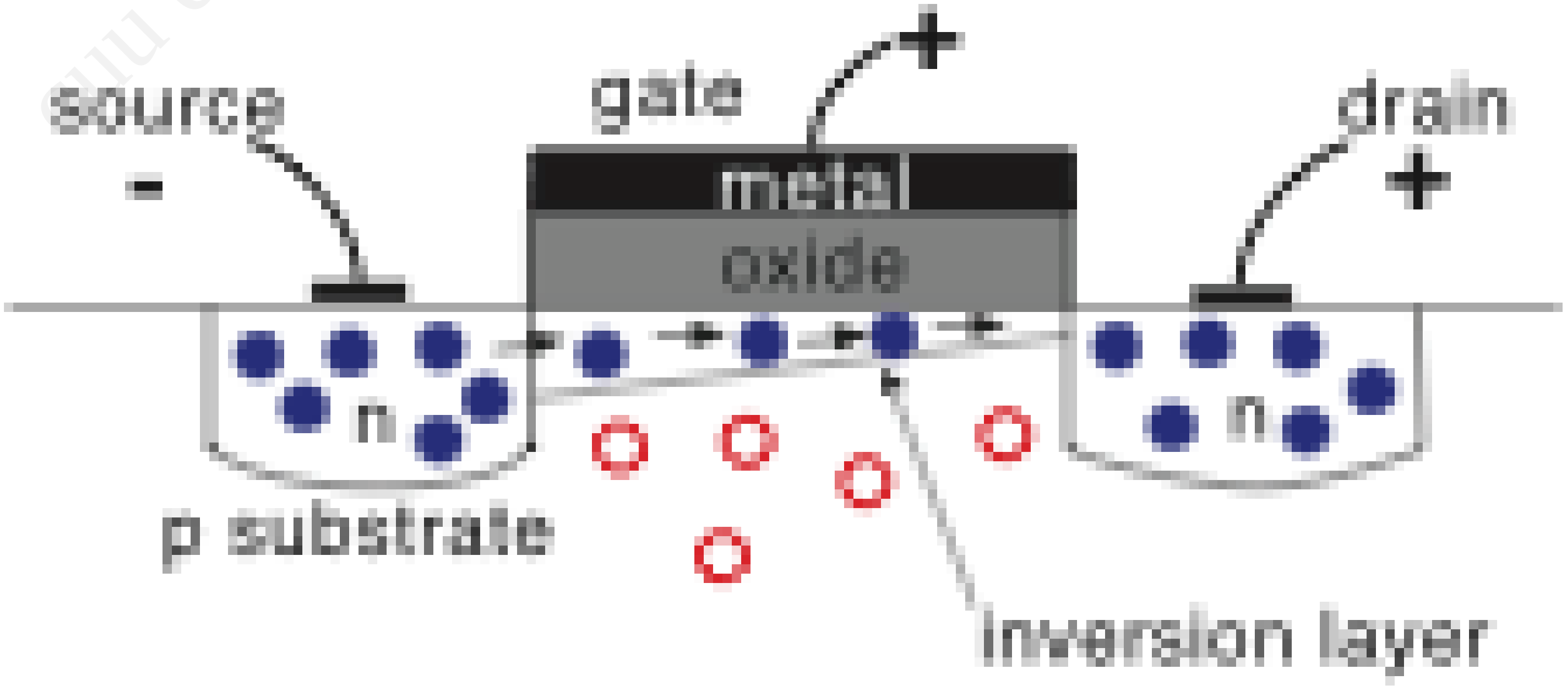
The Metal Oxide Field Effect Transistor (MOSFET)



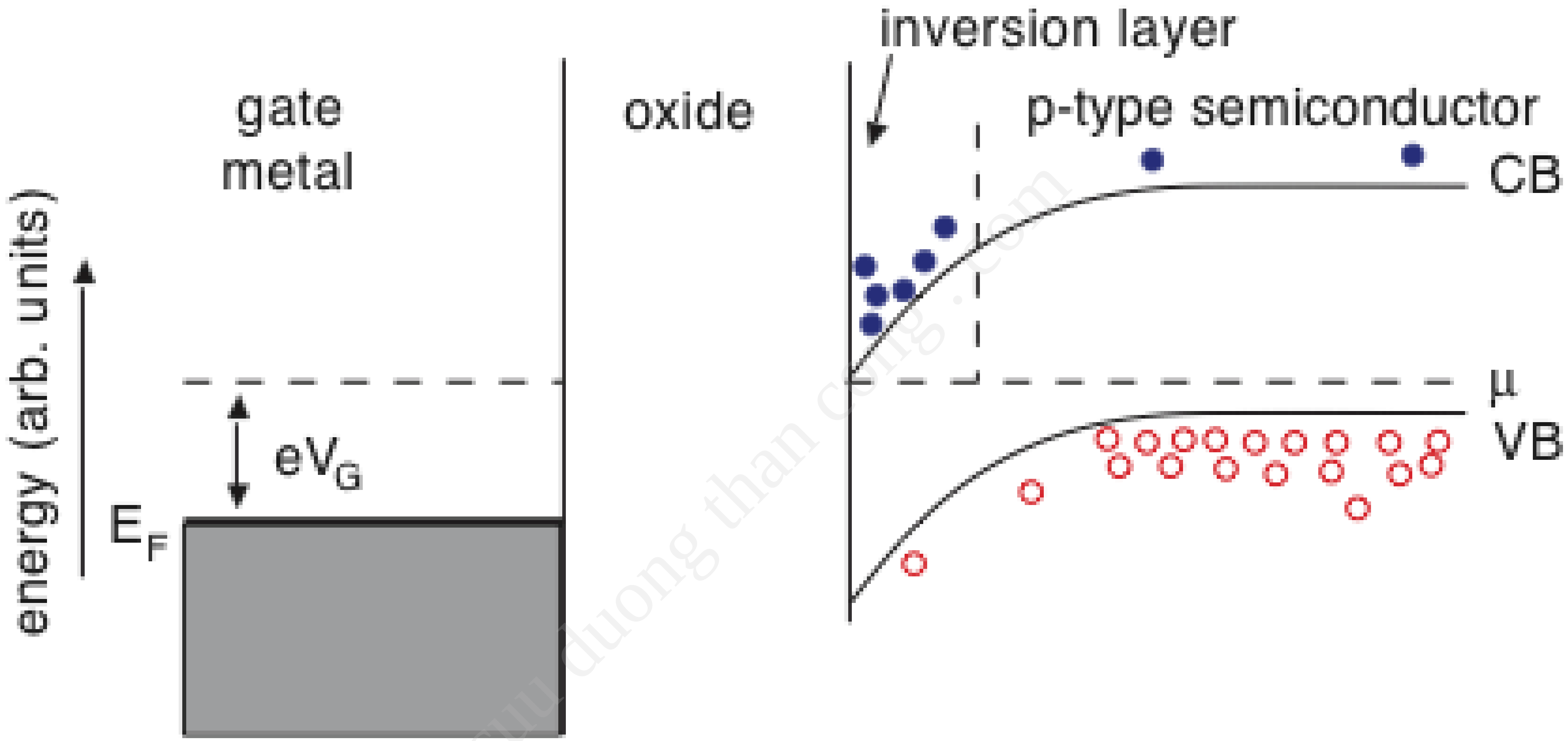
The field effect transistor: principle of operation



$U_{gate} > U_{threshold}$

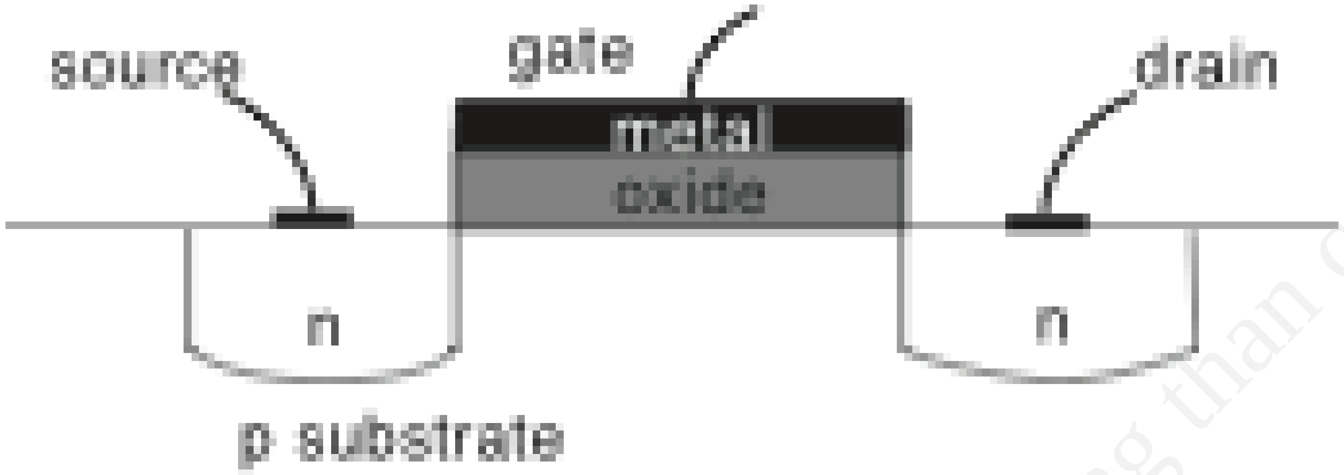


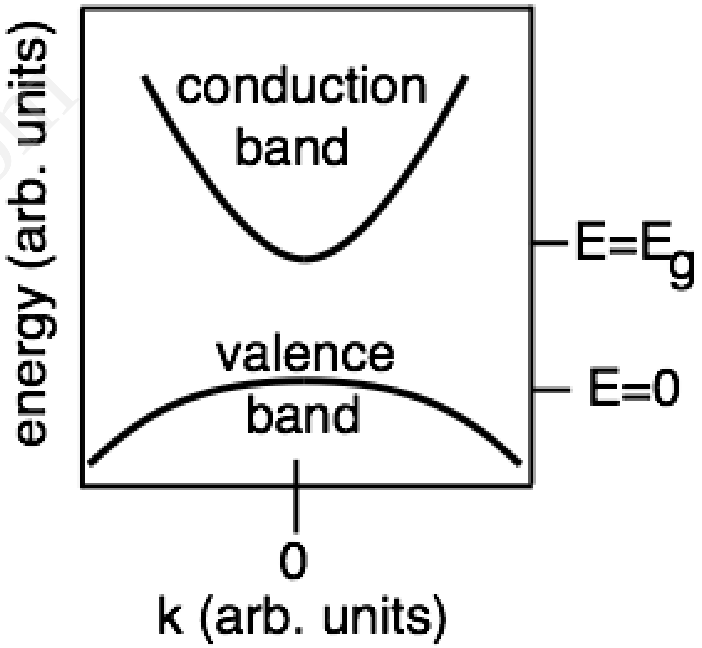
The field effect transistor: principle of operation



- The gate voltage induces a band-bending close to the interface.
- For a sufficiently high voltage, the CB is closer to the chemical potential than the VB and the semiconductor shows n-type behavour.

The field effect transistor

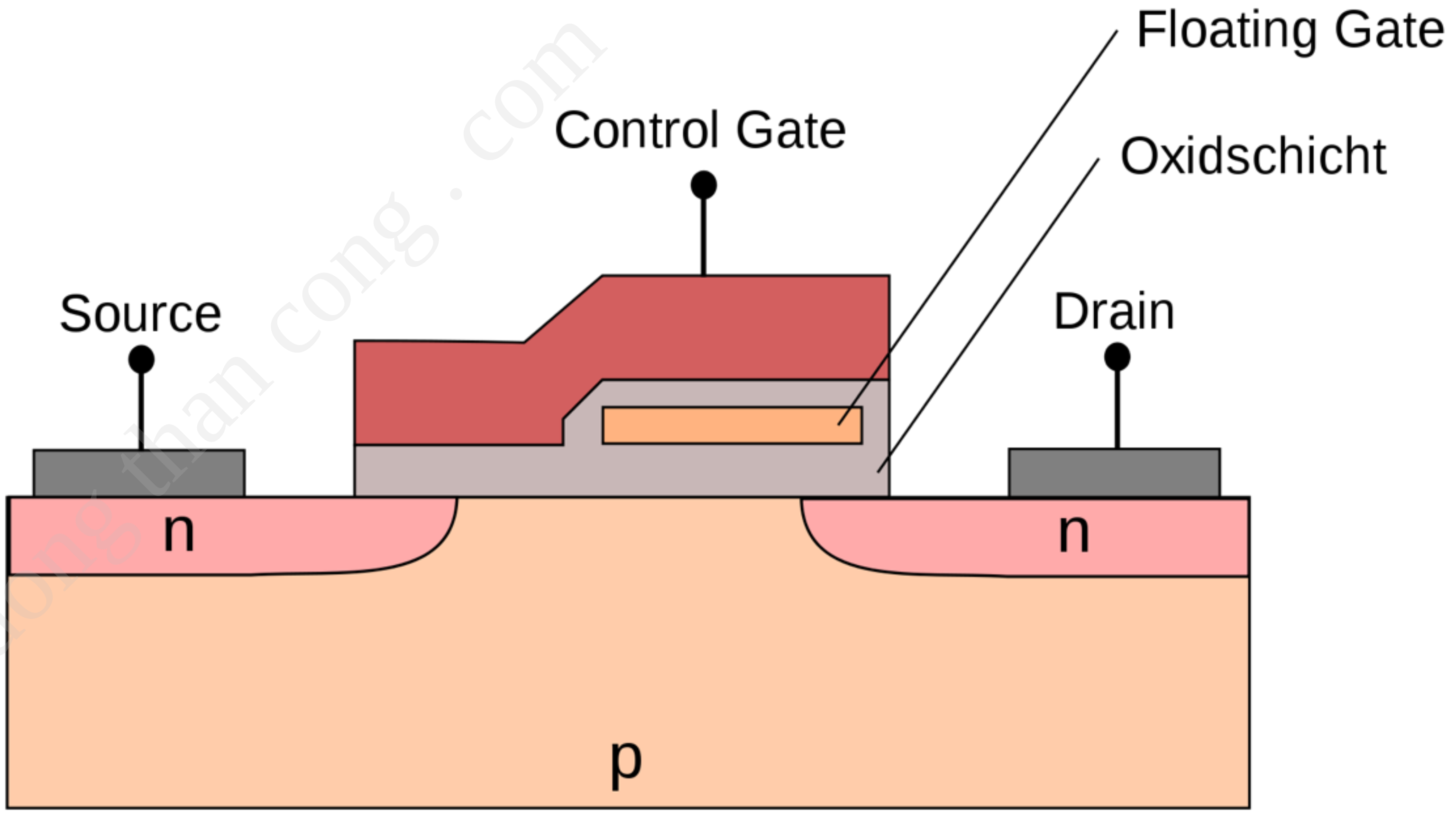




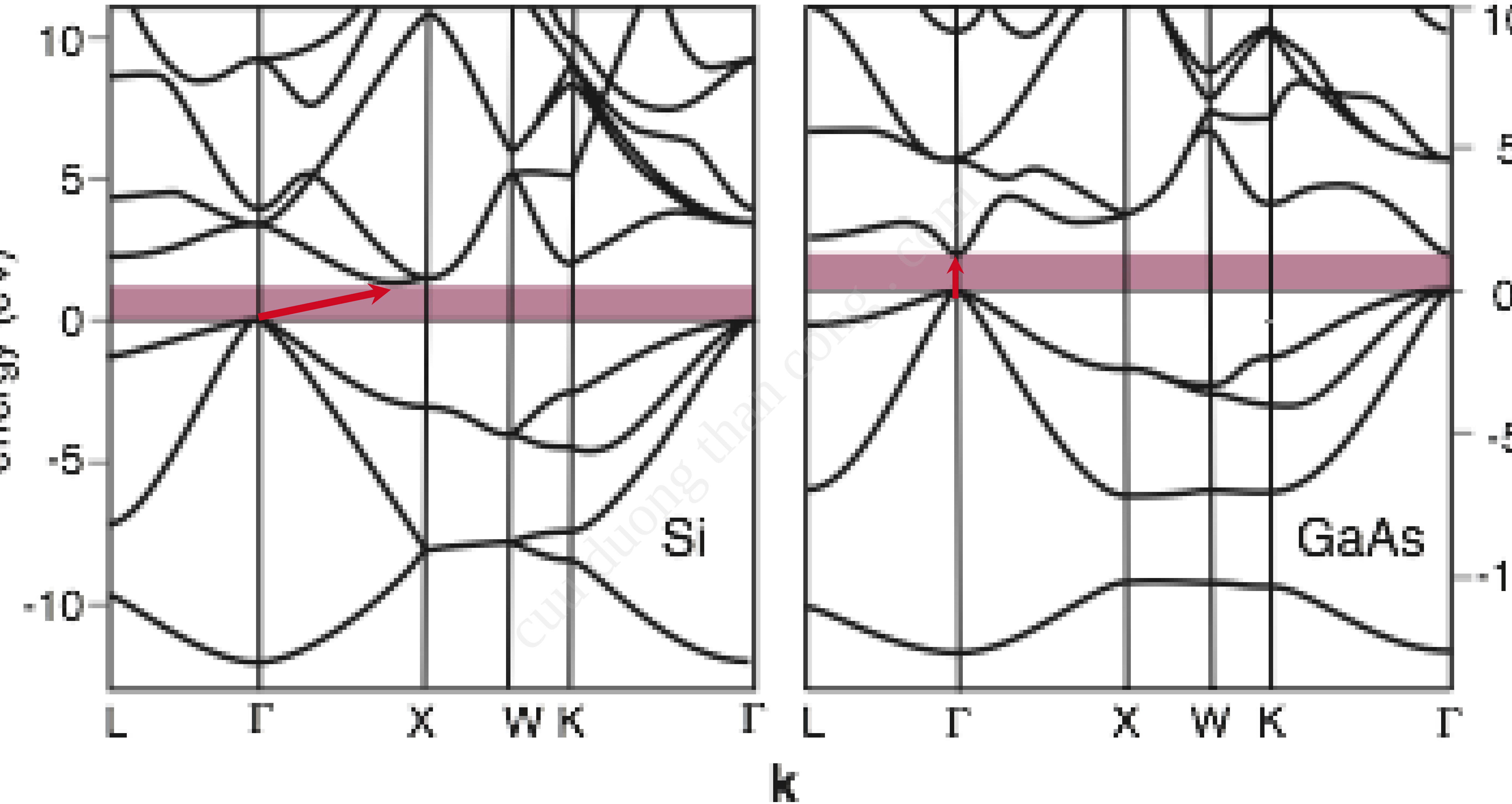
- pnp MOSFETs are also possible but they have the disadvantage that the current is carried by the holes.
- Holes tend to be heavier than electrons in most semiconductors. Remember Britney!

solid state hard drives
flash memory

- most SSD’s are packaged flash memory
- introduced in 1978 and used in some Apple products in the early 80‘ies
- fast, non-volatile, capacity of 1 TB on 3.5’ disc



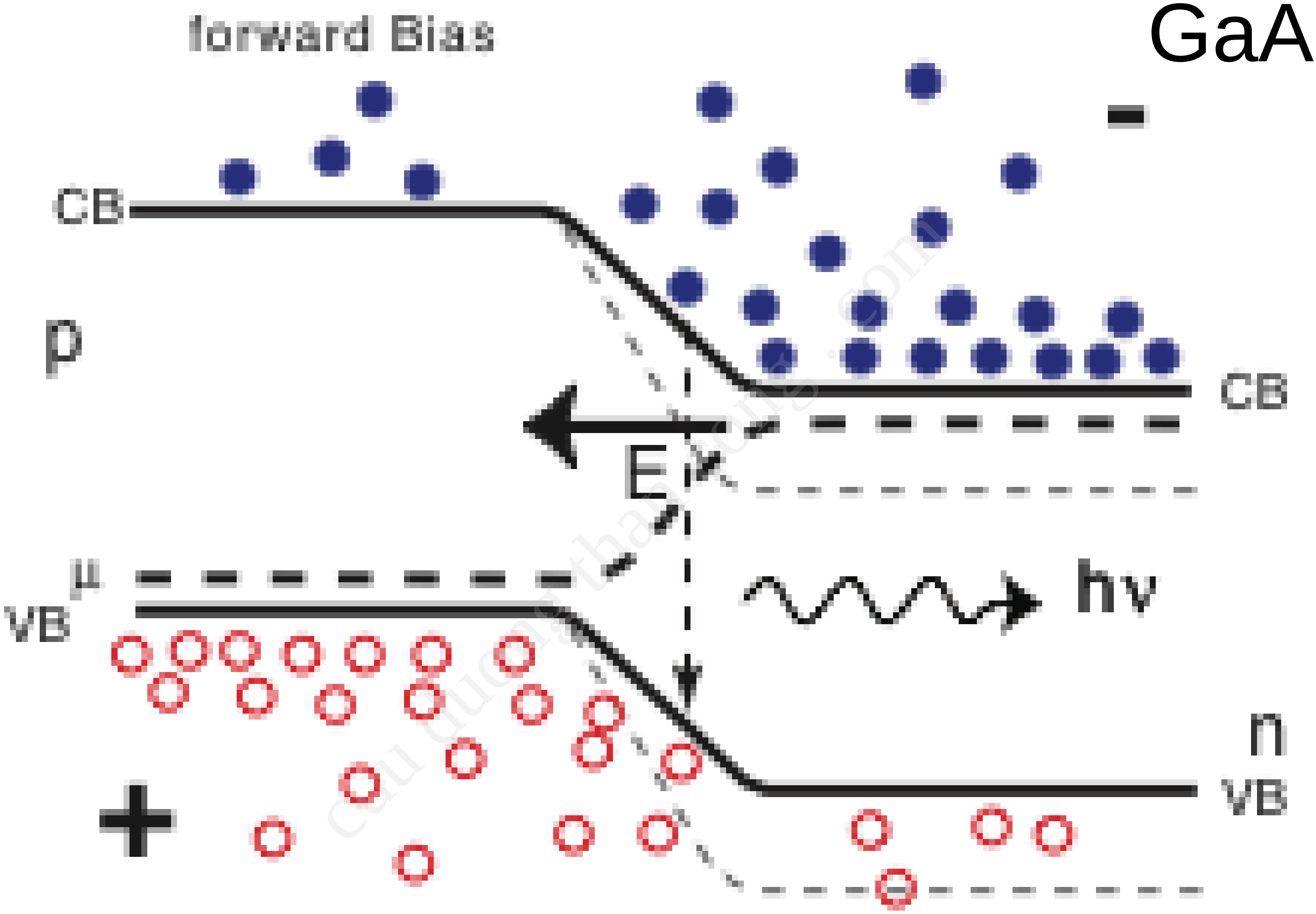
Optical properties



- Optical photons carry energy but almost no momentum.
- A transition with a change in k can therefore not be achieved.

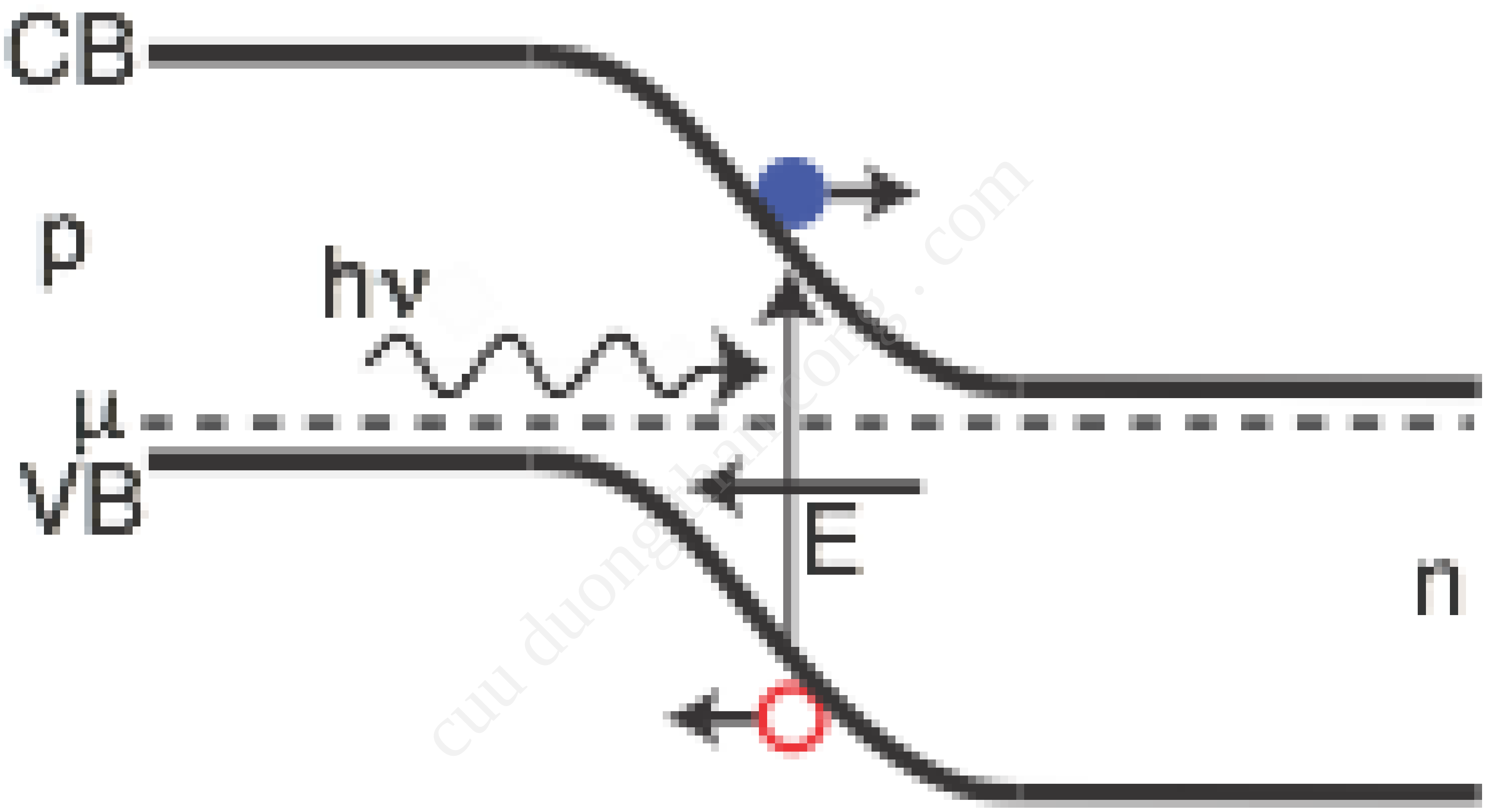
Light emitting diodes (LED)

GaAsP



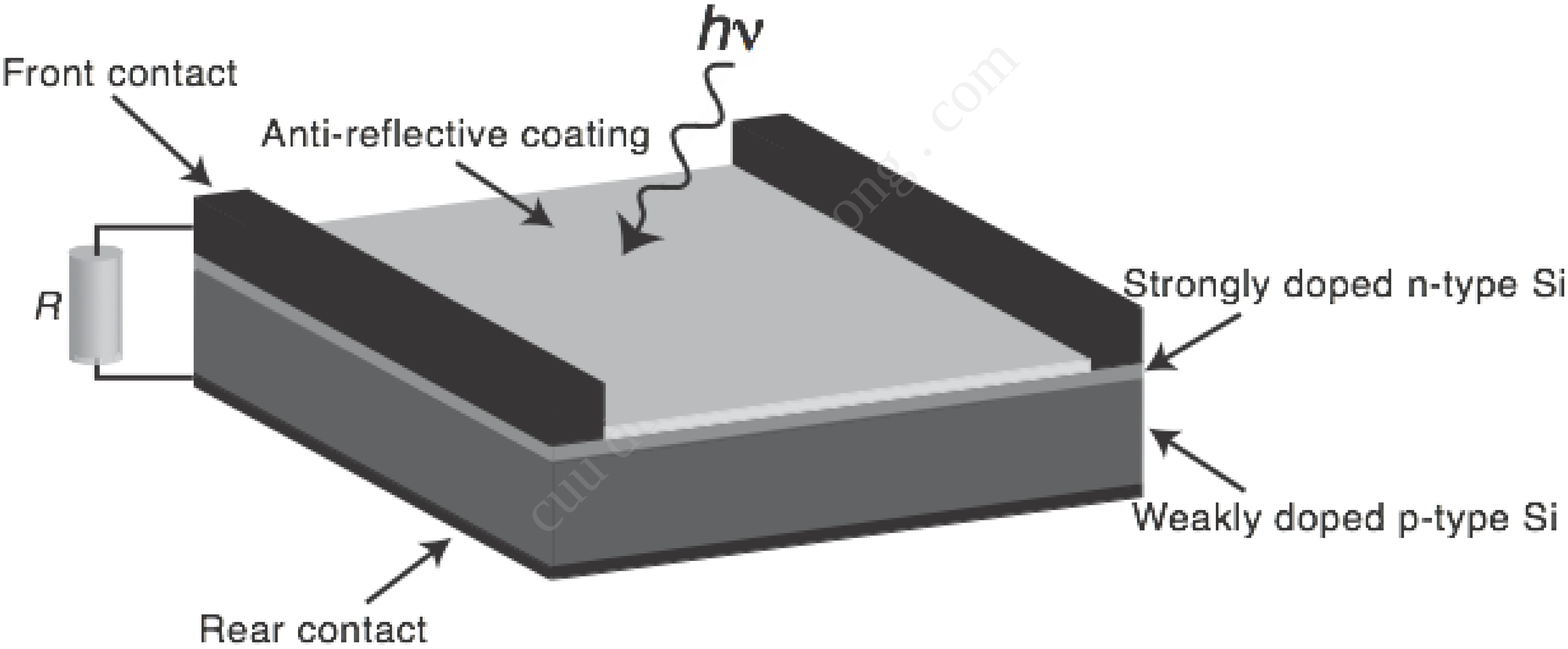
- p-n junction of direct band gap semiconductor operated in forward bias.
- recombination leads to light emission, colour given by band gap.

Solar cell



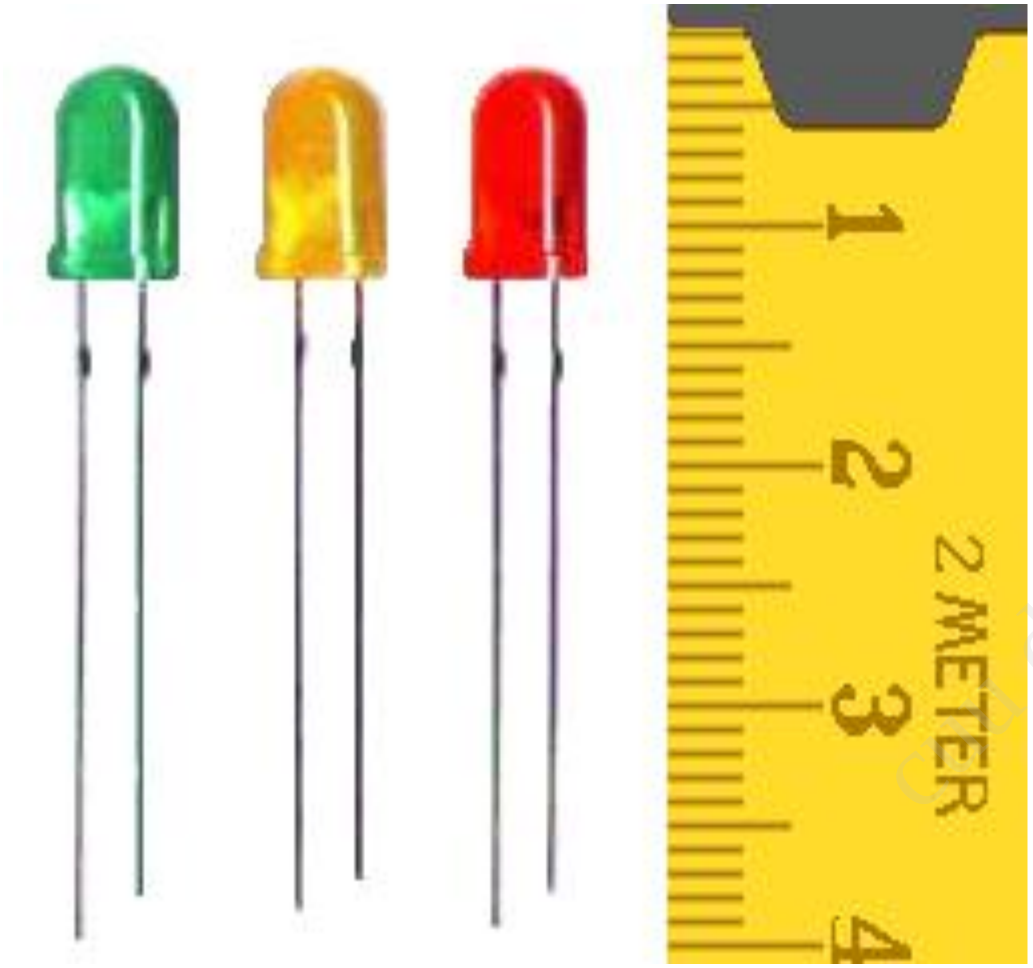
- light induced voltage (current) for reverse-biased diode

Solar cell



hν
Front contact
Anti-reflective coating
R
Strongly doped n-type Si
Weakly doped p-type Si
Rear contact

Light emitting diodes (LED)



efficiency:

> 70 lumens / watt

a “normal” incandescent lamp

around 10 lumens / watt