CHAPTER 2
ENERGY BANDS AND EFFECTIVE MASS

- Semiconductors, insulators and metals
- Semiconductors
- Insulators
- Metals
- The concept of effective mass

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Semiconductors, Insulators and Metals

The electrical properties of metals and insulators are well known to all of us.

Everyday experience has already taught us a lot about the electrical properties of metals and insulators.

But the same cannot be said about "semiconductors".

What happens when we connect a battery to a piece of a silicon;

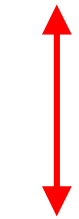
would it conduct well ? or

would it act like an insulator ?

The name “semiconductor” implies that it conducts somewhere between the two cases (conductors or insulators)

Conductivity : σ

$\sigma_{metals} \sim 10^{10}\ /\Omega\text{-cm}$

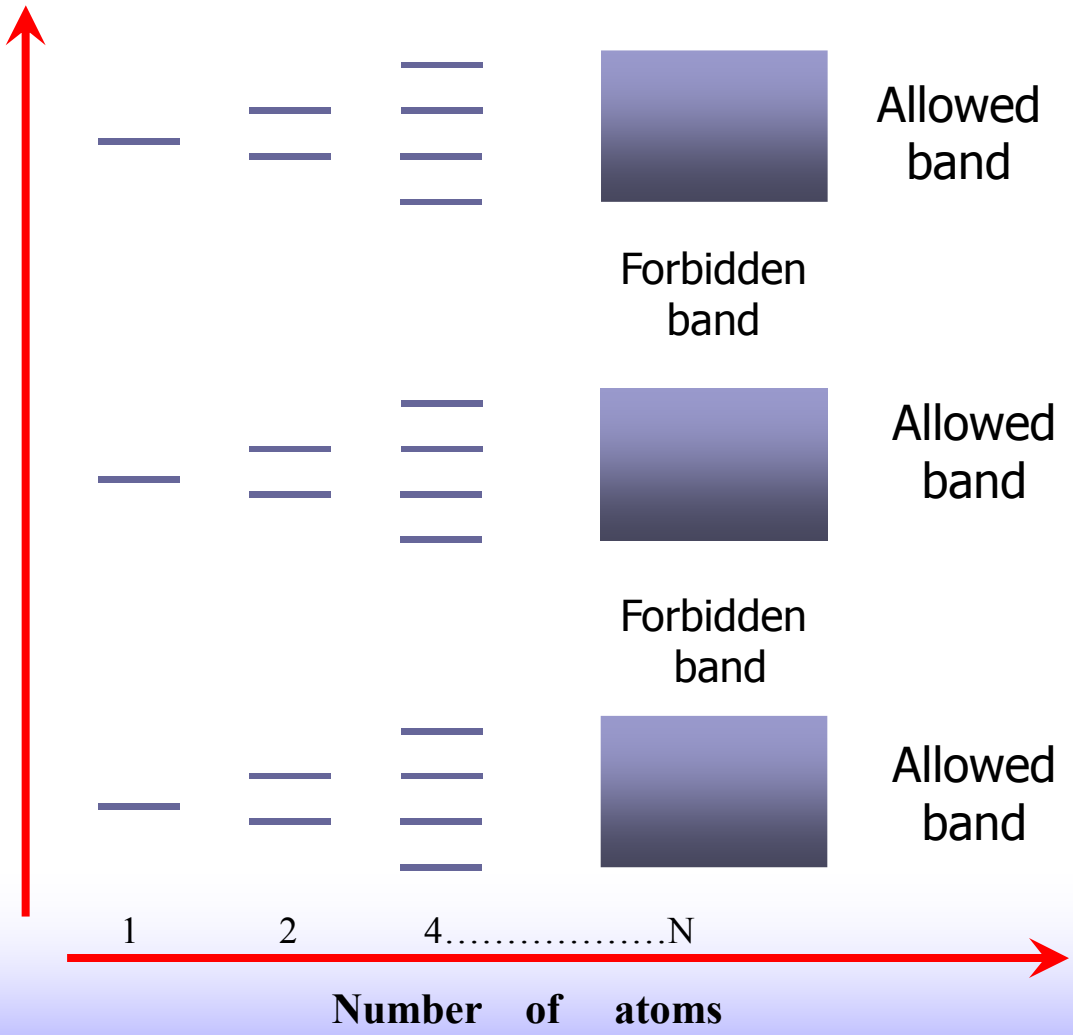


S/C

$\sigma_{insulators} \sim 10^{-22}\ /\Omega\text{-cm}$

The conductivity (σ) of a semiconductor (S/C) lies between these two extreme cases.

.:: The Band Theory of Solids ::.



- The electrons surrounding a nucleus have certain well-defined energy-levels.
- Electrons don't like to have the same energy in the same potential system.
- The most we could get together in the same energy-level was two, provided thet they had opposite spins. This is called *Pauli Exclusion Principle.*

- The difference in energy between each of these smaller levels is so tiny that it is more reasonable to consider each of these sets of smaller energy-levels as being continuous *bands* of energy, rather than considering the enormous number of discrete individual levels.

- Each *allowed band* is seperated from another one by a *forbidden band*.

- Electrons can be found in *allowed bands* but they can not be found in *forbidden bands*.

.:: CALCULATION

- ***Consider 1 cm^3 of Silicon. How many atoms does this contain ?***
- Solution:

The atomic mass of silicon is 28.1 g which contains Avagadro's number of atoms.

Avagadro's number N is 6.02×10^{23} atoms/mol .

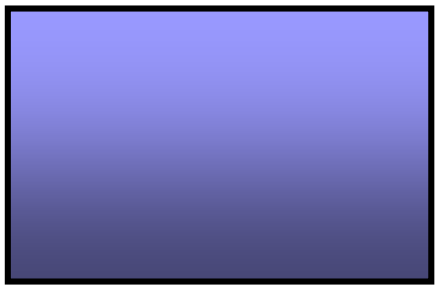
The density of silicon: 2.3×10^3 kg/m^3

so 1 cm^3 of silicon weighs 2.3 gram and so contains

$$\frac{6.02 \times 10^{23}}{28.1} \times 2.3 = 4.93 \times 10^{22}\ atoms$$

This means that in a piece of silicon just one cubic centimeter in volume , each electron energy-level has split up into 4.93×10^{22} smaller levels !

.:: Semiconductor, Insulators, Conductors ::.



Full band

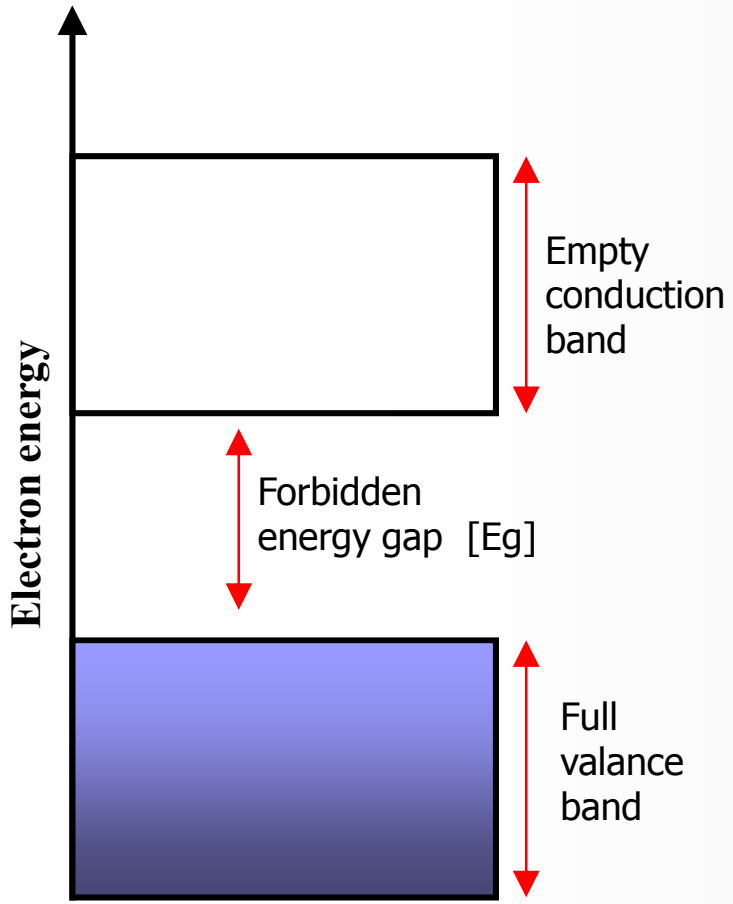
All energy levels are occupied by electrons

Empty band

All energy levels are empty (no electrons)

Both full and empty bands do not partake in electrical conduction.

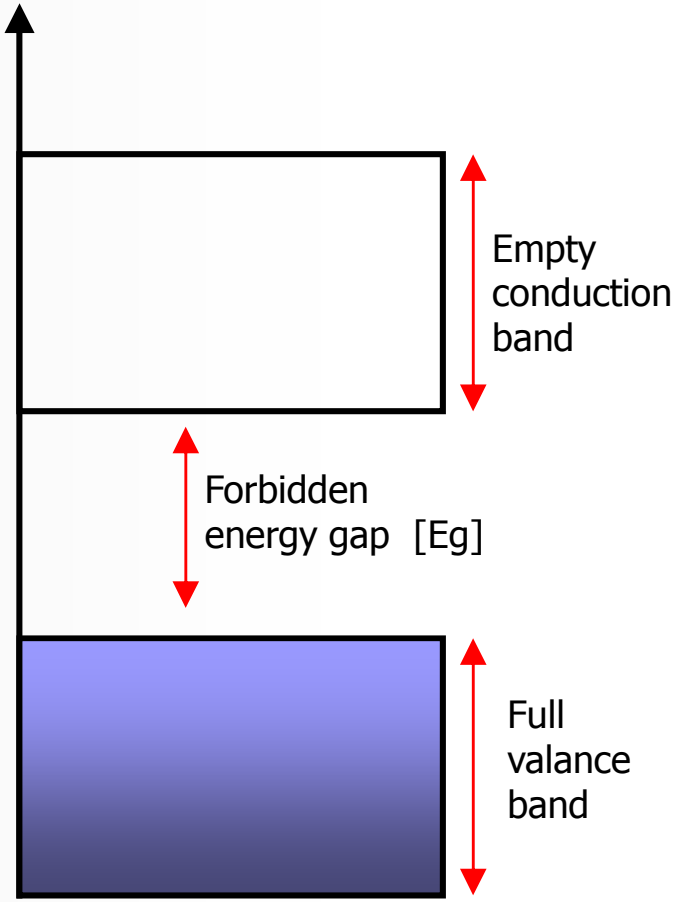
.:: Semiconductor energy bands at low temperature ::.



- At low temperatures the valance band is *full*, and the conduction band is empty.
- Recall that a full band can not conduct, and neither can an empty band.
- At low temperatures, s/c's do not conduct, they behave like insulators.
- The *thermal energy* of the electrons sitting at the top of the full band is much lower than that of the *Eg at low temperatures*.

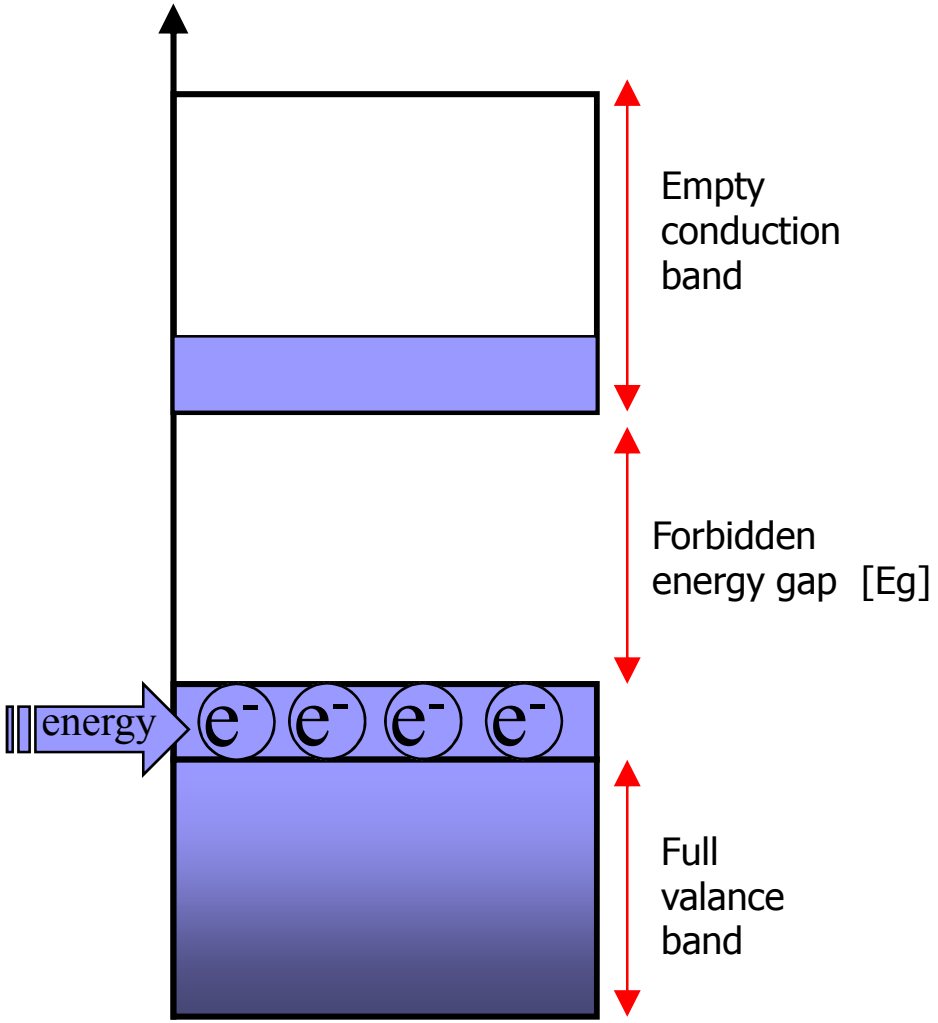
Conduction Electron :

- Assume some kind of energy is provided to the electron (valence electron) sitting at the top of the *valance band.*
- This electron gains energy from the applied field and it would like to move into higher energy states.
- This electron contributes to the *conductivity* and this electron is called as a *conduction electron*.
- At 0^0K, electron sits at the lowest energy levels. The valance band is the highest filled band at zero kelvin.



Semiconductor energy bands at room temperature

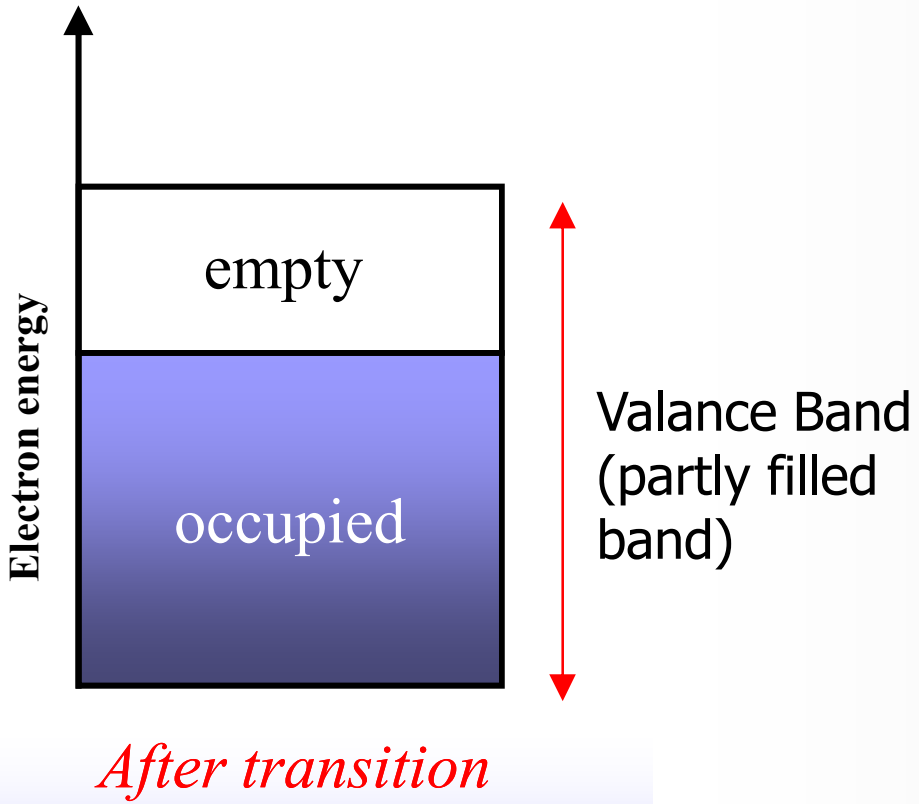
- When enough *energy* is supplied to the e^- sitting at the top of the valance band, e^- can make a transition to the bottom of the conduction band.
- When electron makes such a transition it leaves behind a *missing electron state.*
- This missing electron state is called as a *hole.*
- Hole behaves as a *positive charge carrier.*
- Magnitude of its charge is the same with that of the electron but with an opposite sign.



Conclusions ::.

- Holes contribute to current in *valance band* (VB) as e^-'s are able to create current in *conduction band* (CB).
- Hole is *not* a free particle. It can only exist within the crystal. A hole is simply a vacant electron state.
- A transition results an equal number of e^- in CB and holes in VB. This is an important property of *intrinsic,* or *undoped s/c's*. For *extrinsic*, or *doped*, semiconductors this is no longer true.

Bipolar (two carrier) conduction



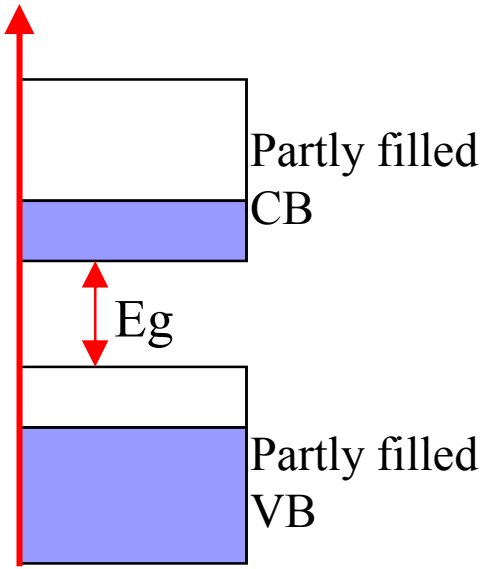
After transition

- *After transition*, the valance band is now no longer full, it is *partly filled* and may conduct electric current.
- The *conductivity* is due to both electrons and holes, and this device is called a *bipolar conductor* or *bipolar device.*

What kind of excitation mechanism can cause an e^- to make a transition from the top of the valance band (VB) to the minimum or bottom of the conduction band (CB) ?

Answer :

- Thermal energy ?
- Electrical field ?
- Electromagnetic radiation ?



Energy band diagram of a s/c at a finite temperature.

To have a partly field band configuration in a s/c , one must use one of these excitation mechanisms.

1-Thermal Energy :

Thermal energy = *k* x *T* = 1.38 x 10^{-23} J/K x 300 K =25 meV

Excitation rate = *constant* x *exp(-Eg / kT)*

Although the thermal energy at room temperature, *RT,* is very small, *i.e.* 25 meV, a few electrons can be promoted to the *CB*.

Electrons can be promoted to the CB by means of thermal energy.

This is due to the exponential increase of excitation rate with increasing temperature.

Excitation rate is a strong function of temperature.

2- Electric field :

- For low fields, this mechanism doesn't promote electrons to the CB in common s/c's such as Si and GaAs.

- An electric field of 10^{18} V/m can provide an energy of the order of 1 eV. This field is enormous.

So , the use of the electric field as an excitation mechanism is not useful way to promote electrons in s/c's.

3- Electromagnetic Radiation :

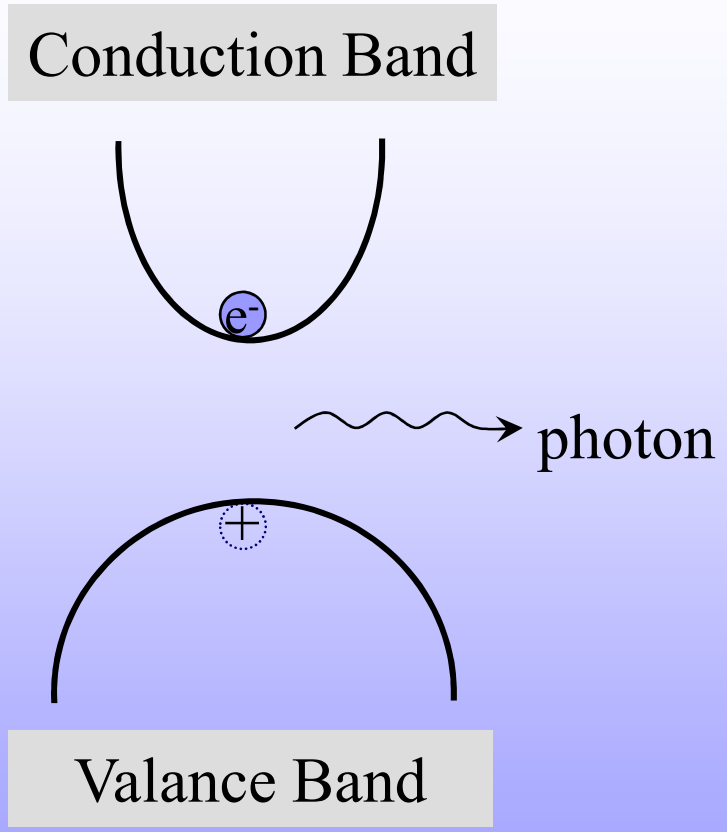
$$E = h\nu = h\frac{c}{\lambda} = (6.62x10^{-34}\,J-s)x(3x10^{8}\,m/s)/\lambda(m) \Rightarrow E(eV) = \frac{1.24}{\lambda(\text{in}\,\mu m)}$$

$h = 6.62 \times 10^{-34}$ J-s
$c = 3 \times 10^{8}$ m/s
1 eV=1.6x10^{-19} J

$$for \quad \text{Silicon} \quad E_g = 1.1eV \qquad \lambda(\mu m) = \frac{1.24}{1.1} = 1.1\mu m$$

Near infrared

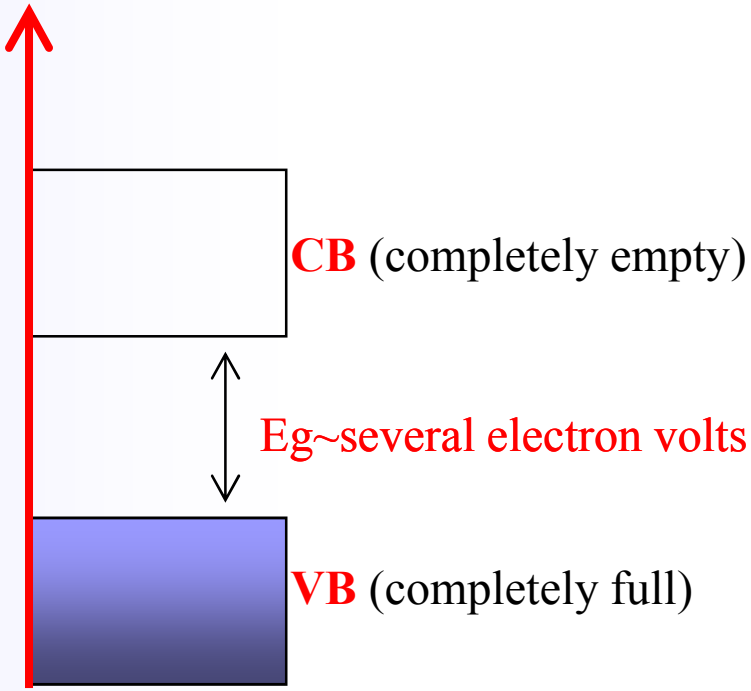
To promote electrons from VB to CB Silicon , the wavelength of the photons must 1.1 μm or less



- The converse transition can also happen.
- An electron in CB recombines with a hole in VB and generate a photon.
- The energy of the photon will be in the order of Eg.
- If this happens in a direct band-gap s/c, it forms the basis of LED's and LASERS.

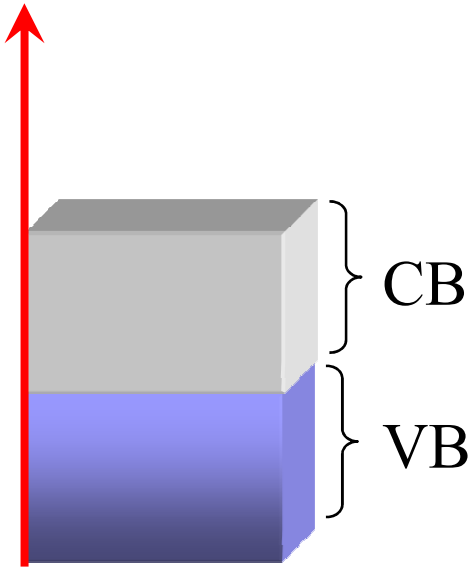
Insulators :

- The magnitude of the band gap determines the differences between insulators, s/c‘s and metals.
- The excitation mechanism of thermal is not a useful way to promote an electron to CB even the melting temperature is reached in an insulator.
- Even very high electric fields is also unable to promote electrons across the band gap in an insulator.

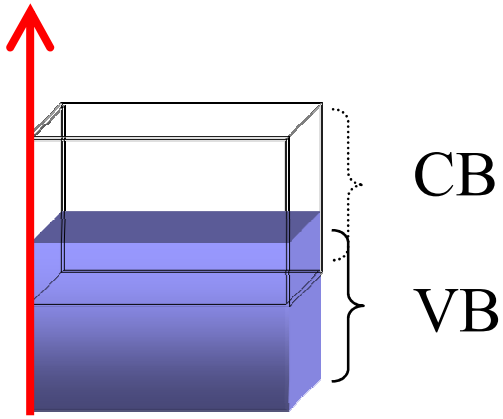


Wide band gaps between VB and CB

Metals :



Touching VB and CB



Overlapping VB and CB

- These two bands looks like as if partly filled bands and it is known that partly filled bands conducts well.
- This is the reason why metals have high conductivity.

- No gap between *valance band* and *conduction band*

The Concept of Effective Mass :

Comparing

Free e^- in vacuum

In an electric field

↓

$m_o = 9.1 \times 10^{-31}$

↓

Free electron mass

An e^- in a crystal

In an electric field

↓

In a crystal

↓

m = ?

↓

m^* → effective mass

- If the same magnitude of electric field is applied to both electrons in vacuum and inside the crystal, the electrons will accelerate at a different rate from each other due to the existence of different potentials inside the crystal.
- The electron inside the crystal has to try to make its own way.
- So the electrons inside the crystal will have a different mass than that of the electron in vacuum.
- This altered mass is called as an ***effective-mass.***

What is the expression for m^*

- Particles of electrons and holes behave as a wave under certain conditions. So one has to consider the de Broglie wavelength to link partical behaviour with wave behaviour.
- Partical such as electrons and waves can be diffracted from the crystal just as X-rays .
- Certain electron momentum is not allowed by the crystal lattice. This is the origin of the energy band gaps.

$$n\lambda = 2d\sin\theta$$

n = the order of the diffraction
λ = the wavelength of the X-ray
d = the distance between planes
θ = the incident angle of the X-ray beam

$$n\lambda = 2d \qquad (1)$$

The waves are standing waves

$$\lambda = \frac{2\pi}{k}$$

k is the propogation constant

The momentum is

$$P = \hbar k \qquad (2)$$

The energy of the free electron can be related to its momentum

$$E = \frac{P^2}{2m}$$

$P = \frac{h}{\lambda}$

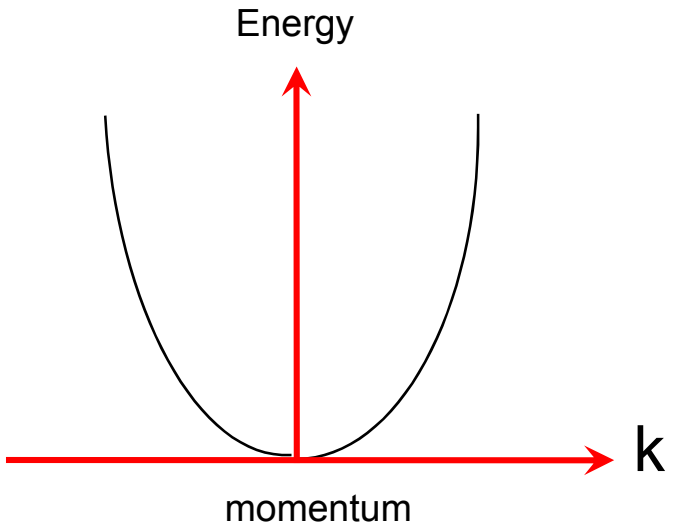
free e$^-$ mass , m_0

$$E = \frac{h^2}{2m}\frac{1}{\lambda^2} = \frac{h^2}{2m}\frac{k^2}{(2\pi)^2}$$

$$\hbar = \frac{h}{2\pi} \qquad E = \frac{\hbar^2 k^2}{2m}$$

The energy of the free e$^-$ is related to the k

By means of equations (1) and (2) certain e$^-$ momenta are not allowed by the crystal. The velocity of the electron at these momentum values is zero.



E versus k diagram is a parabola.

Energy is continuous with k, i,e, all energy (momentum) values are allowed.

E versus k diagram
or
Energy versus momentum diagrams

To find effective mass , m^*

We will take the derivative of *energy* with respect to *k* ;

$$\frac{dE}{dk} = \frac{\hbar^2 k}{m}$$

$$\frac{d^2E}{dk^2} = \frac{\hbar^2}{m}$$

- m^* is determined by the curvature of the E-k curve
- m^* is inversely proportional to the curvature

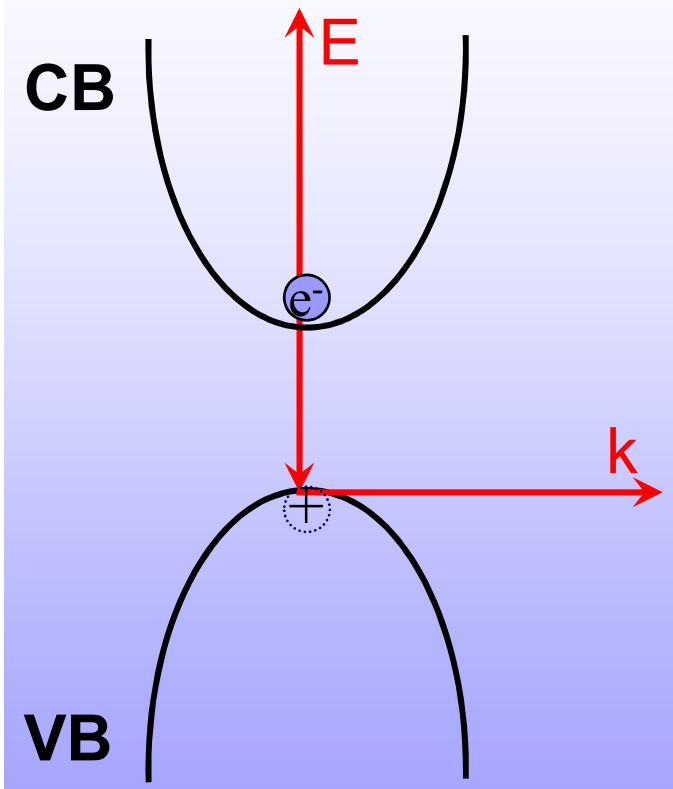
Change m^* instead of m

$$m^* = \frac{\hbar^2}{d^2E/dk^2}$$

This formula is the *effective mass* of an electron inside the crystal.

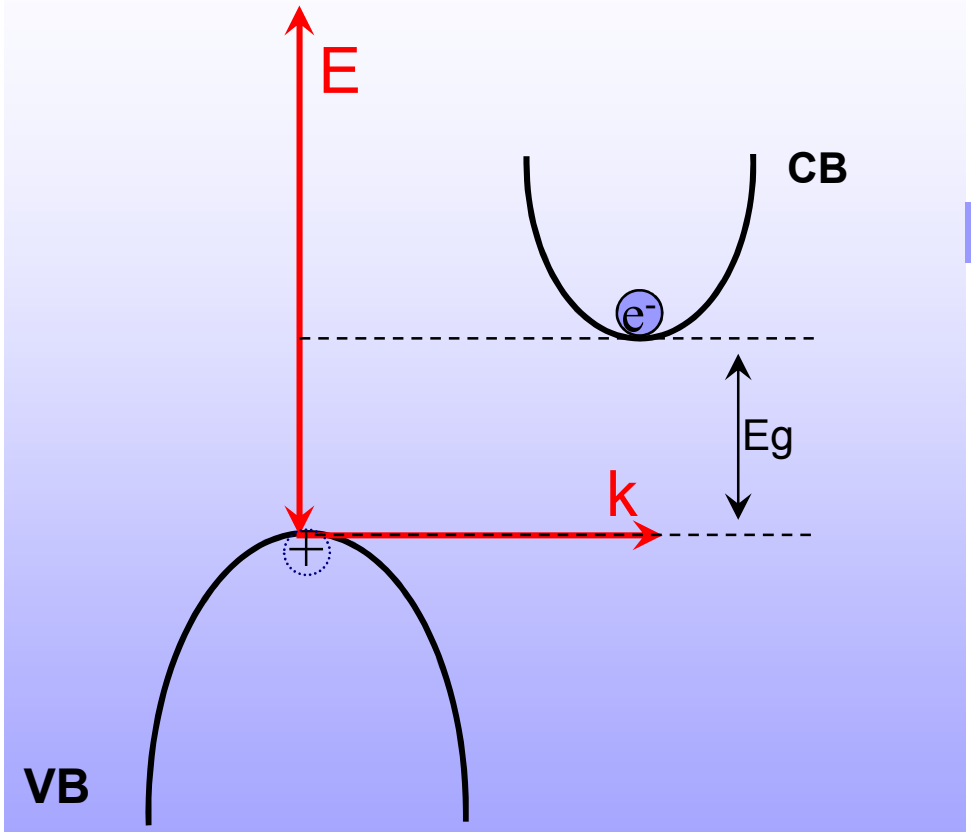
Direct an indirect-band gap materials :

Direct-band gap s/c's (e.g. GaAs, InP, AlGaAs)



- For a *direct-band gap material*, the minimum of the conduction band and maximum of the valance band lies at the same momentum, k, values.
- When an electron sitting at the bottom of the CB recombines with a hole sitting at the top of the VB, there will be no change in momentum values.
- Energy is conserved by means of emitting a photon, such transitions are called as radiative transitions.

Indirect-band gap s/c's (e.g. Si and Ge)



- For an indirect-band gap material; the minimum of the CB and maximum of the VB lie at different k-values.
- When an e^- and hole recombine in an indirect-band gap s/c, phonons must be involved to conserve momentum.

Phonon

- Atoms vibrate about their mean position at a finite temperature.These vibrations produce vibrational waves inside the crystal.
- Phonons are the quanta of these vibrational waves. Phonons travel with a velocity of sound .
- Their wavelength is determined by the crystal lattice constant. Phonons can only exist inside the crystal.

- The transition that involves phonons without producing photons are called *nonradiative (radiationless) transitions*.
- These transitions are observed in an *indirect band gap* s/c and result in inefficient photon producing.
- So in order to have efficient LED's and LASER's, one should choose materials having direct band gaps such as compound s/c's of GaAs, AlGaAs, etc…

.:: CALCULATION

- *For GaAs, calculate a typical (band gap) photon energy and momentum , and compare this with a typical phonon energy and momentum that might be expected with this material.*

photon

E(photon) = Eg(GaAs) = 1.43 ev

E(photon) = h υ = hc / λ

c= 3×10^8 m/sec

P = h / λ h=6.63×10^{-34} J-sec

λ (photon)= 1.24 / 1.43 = 0.88 μm

P(photon) = h / λ = 7.53×10^{-28} kg-m/sec

phonon

E(phonon) = h υ= hv_s / λ

= hv_s / a_0

λ (phonon) ~a_0 = lattice constant =5.65×10^{-10} m

V_s= 5×10^3 m/sec (velocity of sound)

E(phonon) = hv_s / a_0 =0.037 eV

P(phonon)= h / λ = h / a_0 = 1.17×10^{-24} kg-m/sec

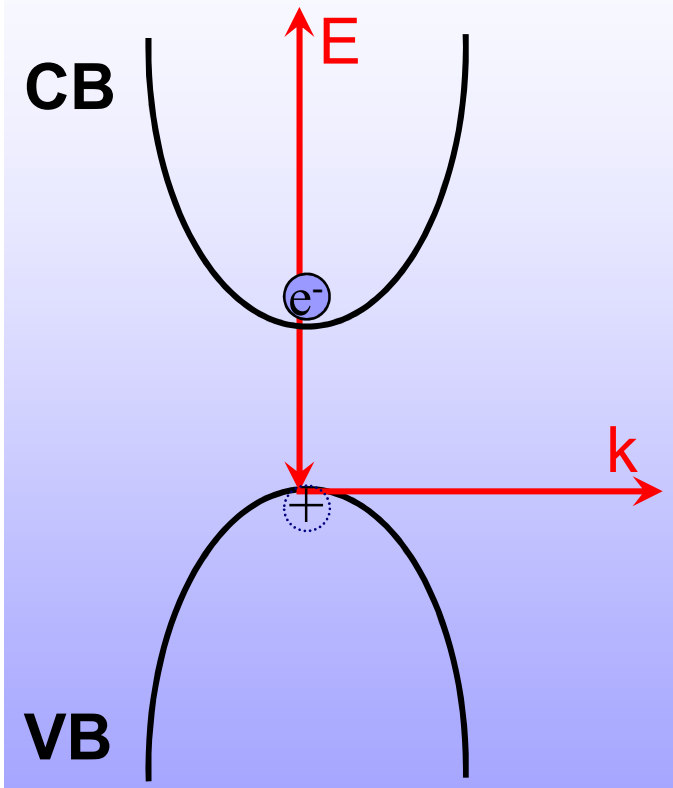
- Photon energy = 1.43 eV
- Phonon energy = 37 meV
- Photon momentum = 7.53×10^{-28} kg-m/sec
- Phonon momentum = 1.17×10^{-24} kg-m/sec

Photons carry large energies but negligible amount of momentum.

On the other hand, phonons carry very little energy but significant amount of momentum.

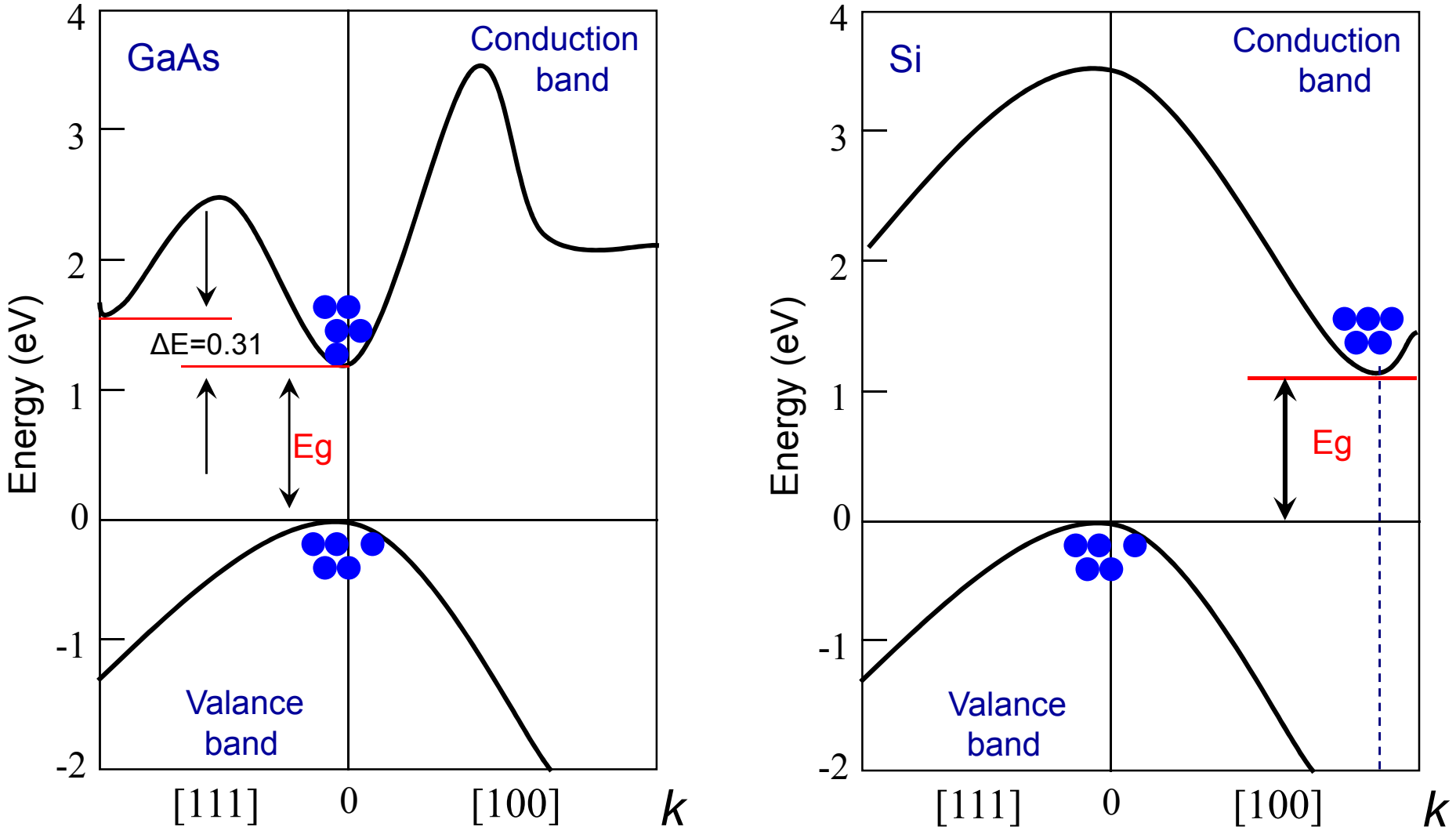
Positive and negative effective mass

Direct-band gap s/c's (e.g. GaAs, InP, AlGaAs)

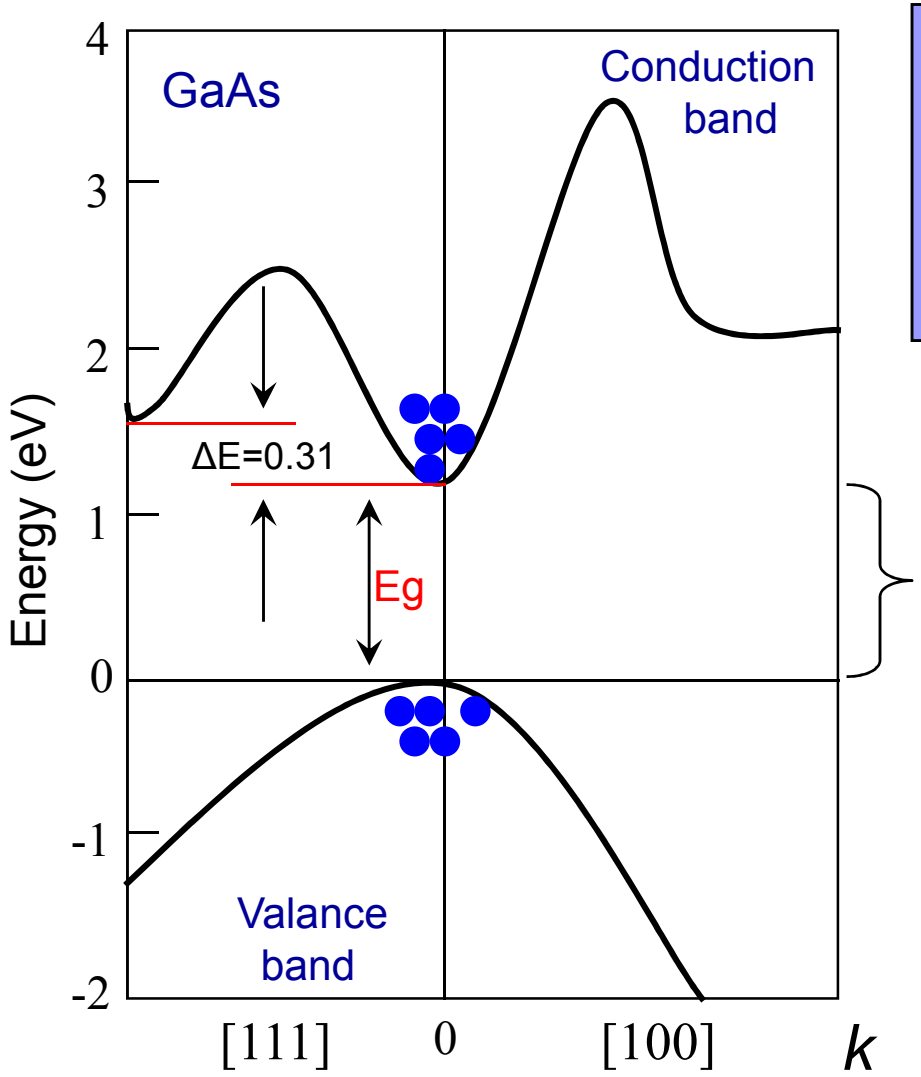


$$m^* = \frac{\hbar^2}{d^2E/dk^2}$$

- The sign of the effective mass is determined directly from the sign of the curvature of the E-k curve.
- The curvature of a graph at a minimum point is a positive quantity and the curvature of a graph at a maximum point is a negative quantity.
- Particles(electrons) sitting near the minimum have a ***positive effective mass***.
- Particles(holes) sitting near the valence band maximum have a ***negative effective mass***.
- A negative effective mass implies that a particle will go ***'the wrong way'*** when an extrernal force is applied.



Energy band structures of *GaAs* and *Si*



Band gap is the smallest energy separation between the valence and conduction band edges.

The smallest energy difference occurs at the same momentum value

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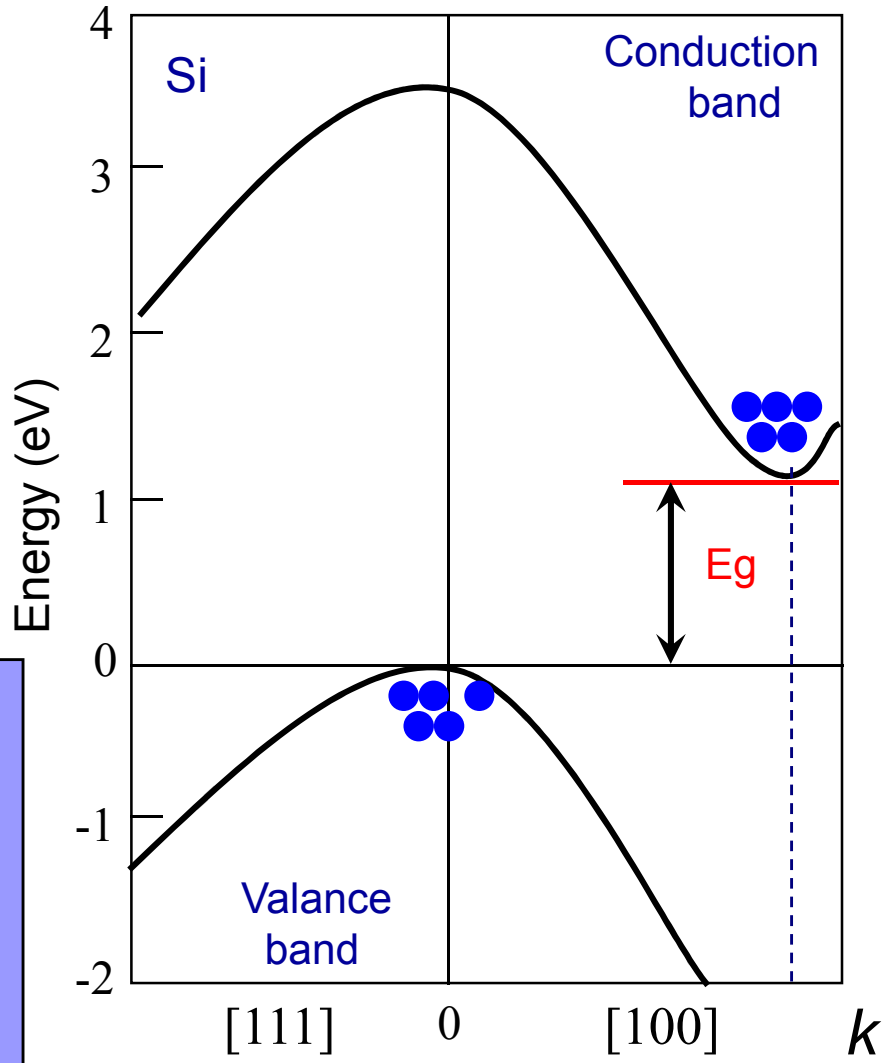
Direct band gap semiconductor

Energy band structure of *GaAs*

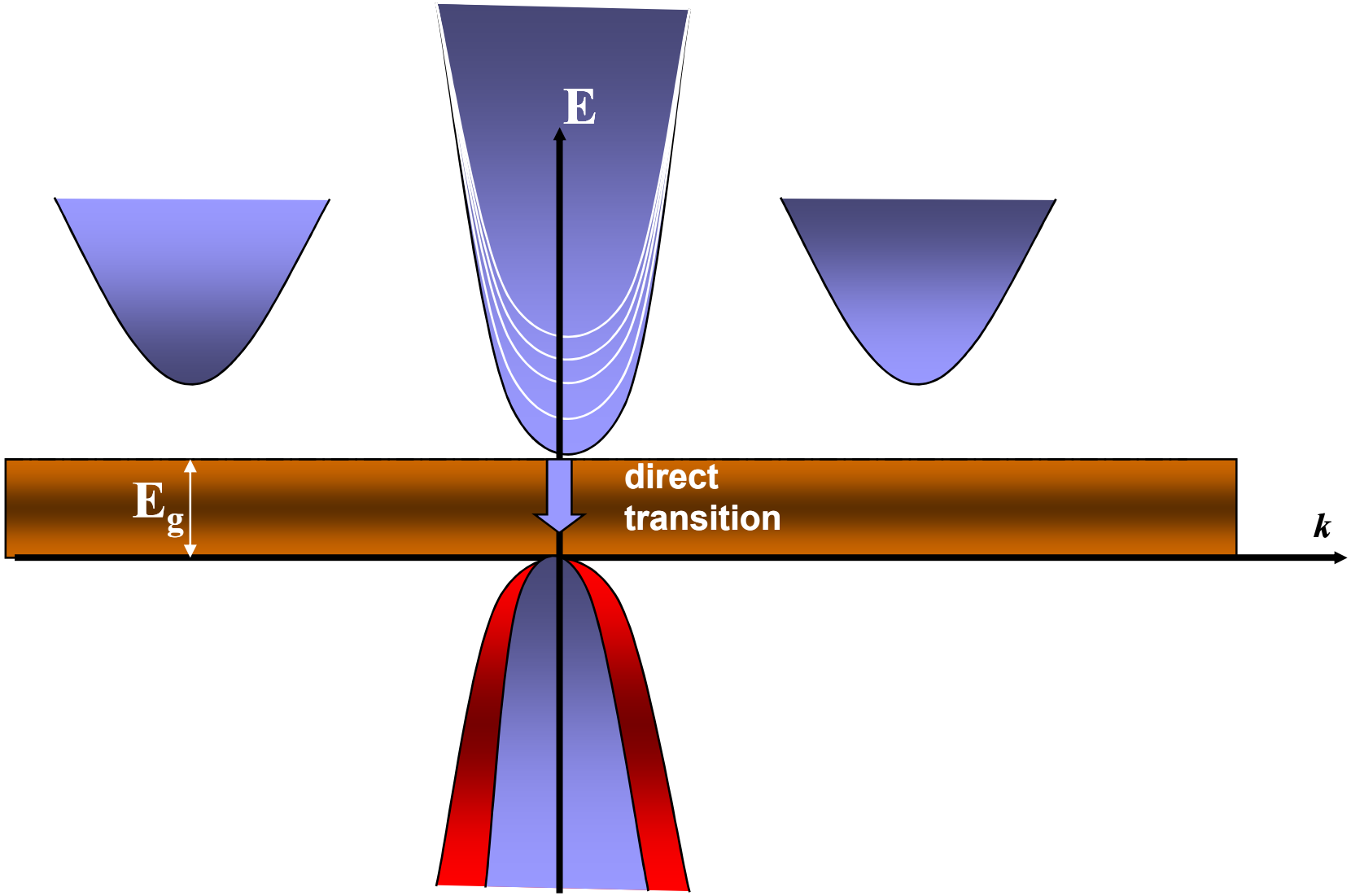
The smallest energy gap is between the top of the VB at k=0 and one of the CB minima away from k=0

Indirect band gap semiconductor



- Band structure of AlGaAs?
- Effective masses of CB satellites?
- Heavy- and light-hole masses in VB?

Energy band structure of *Si*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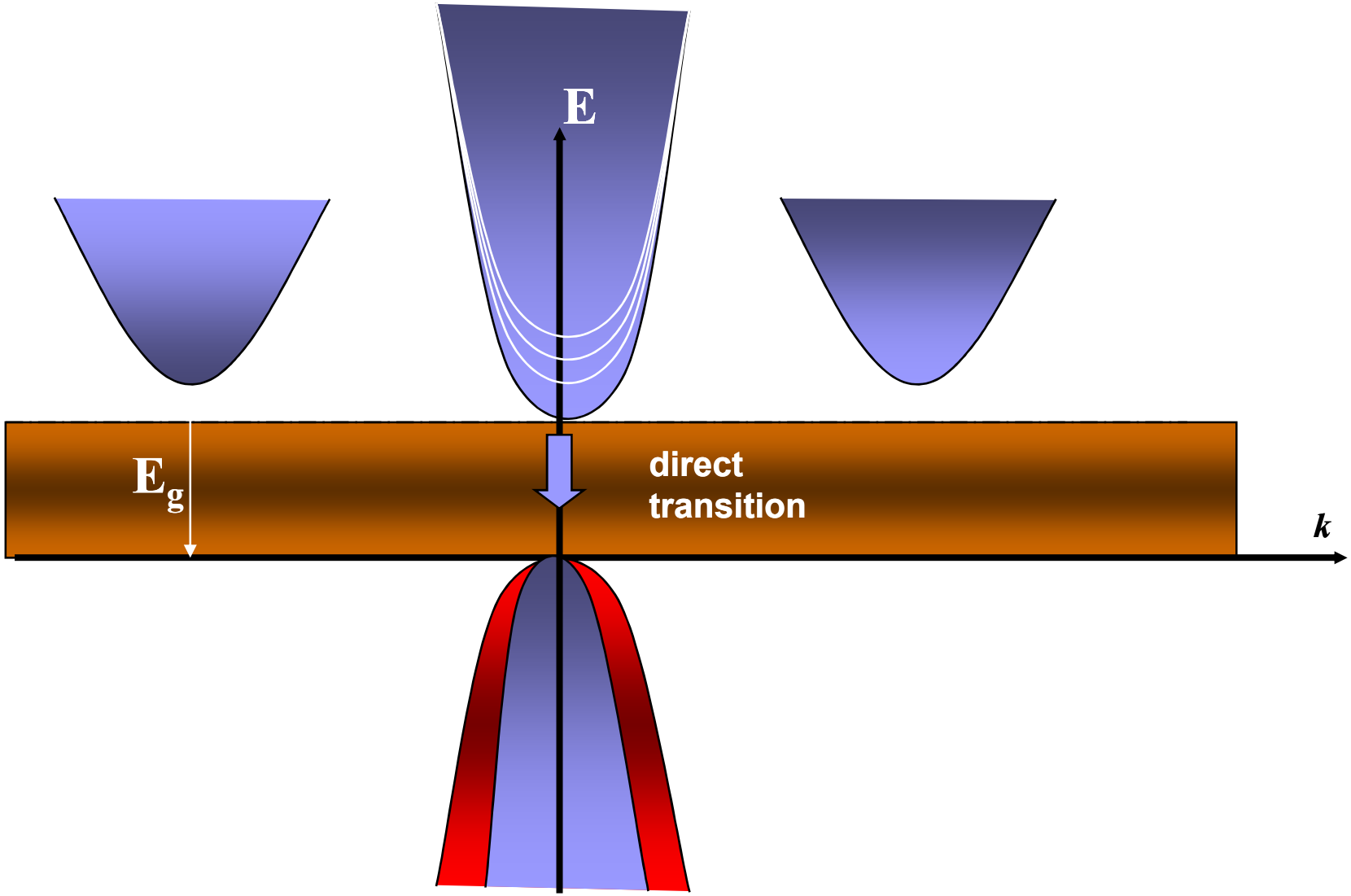
E_g
direct
transition
k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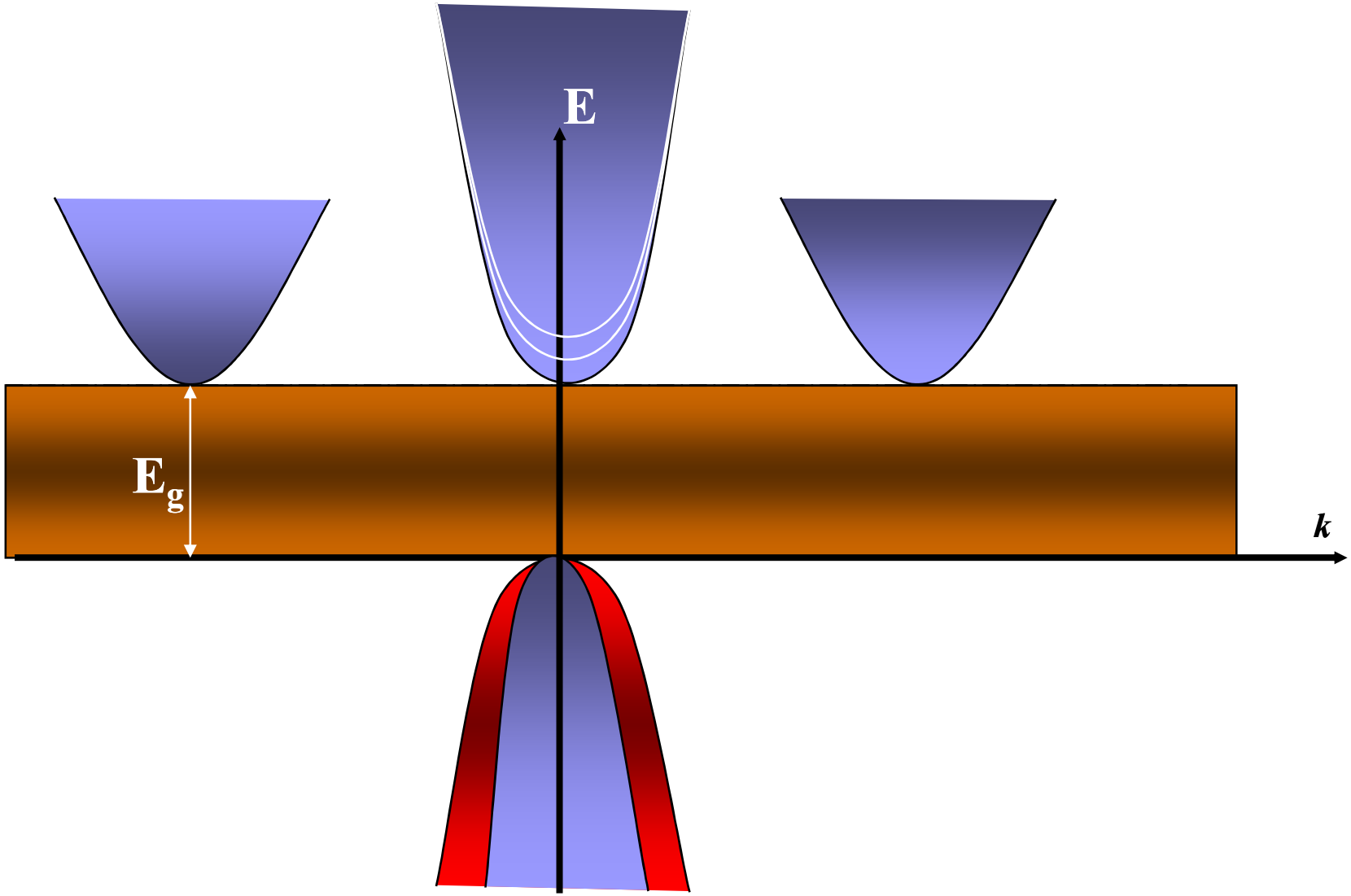
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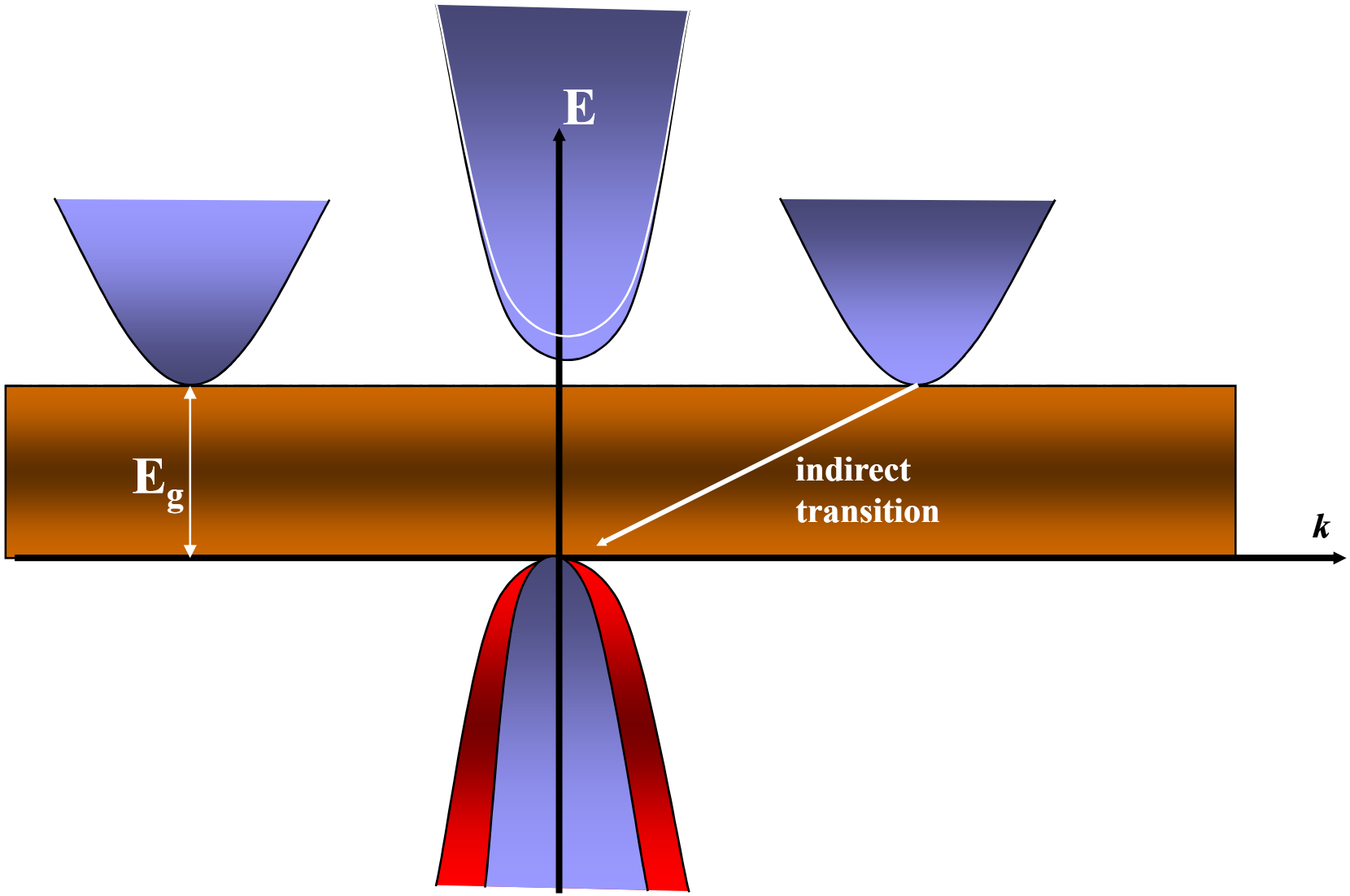
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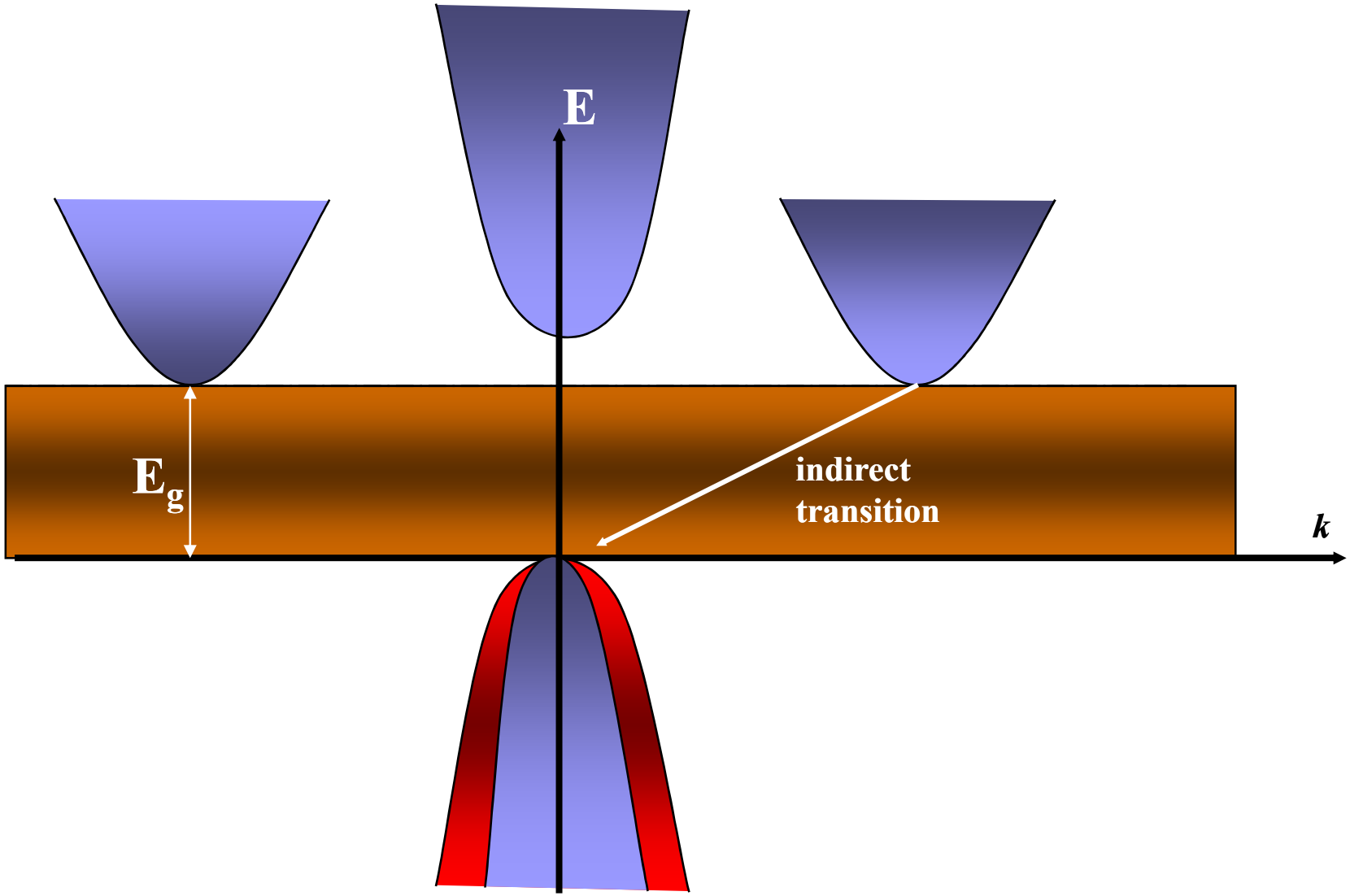
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