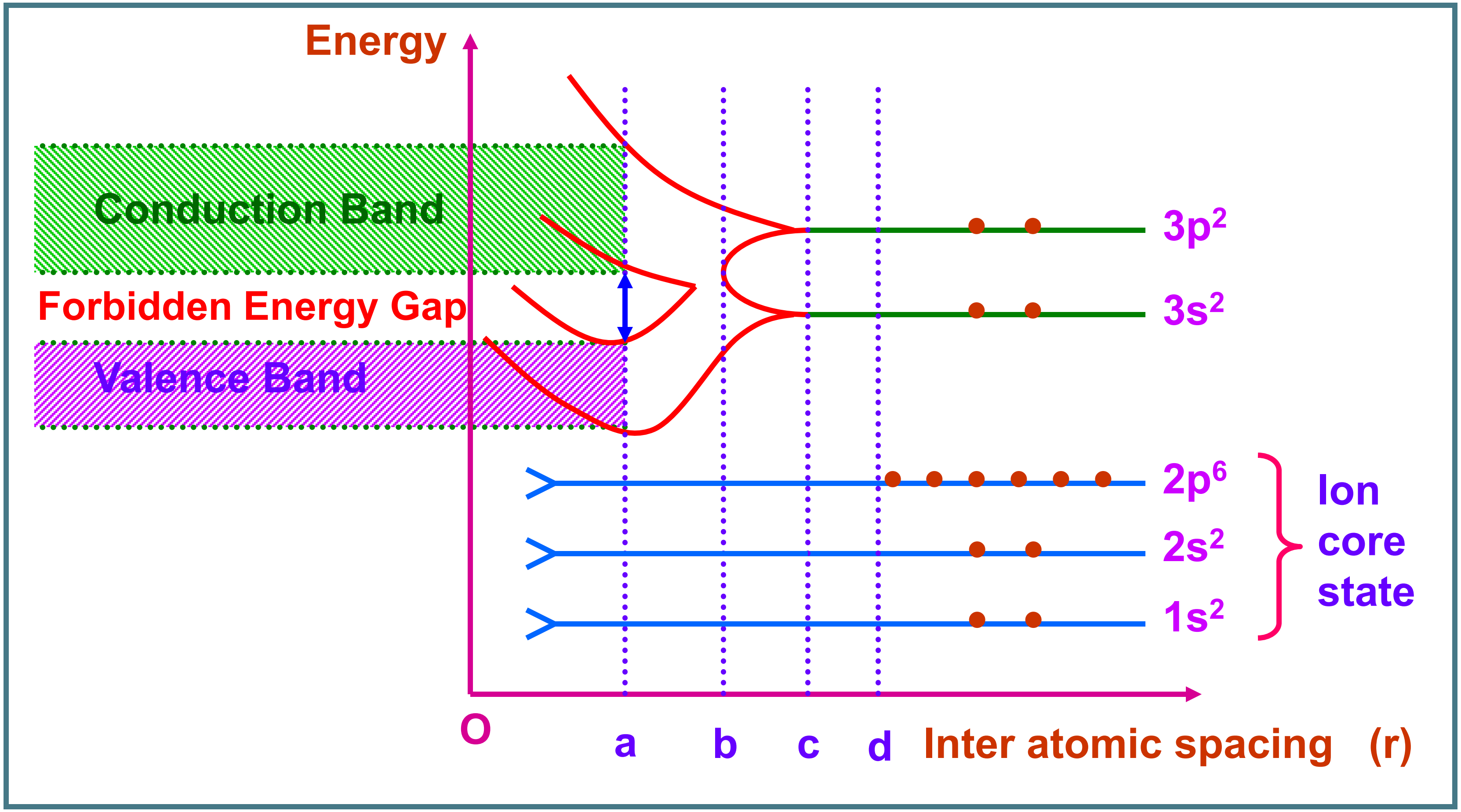
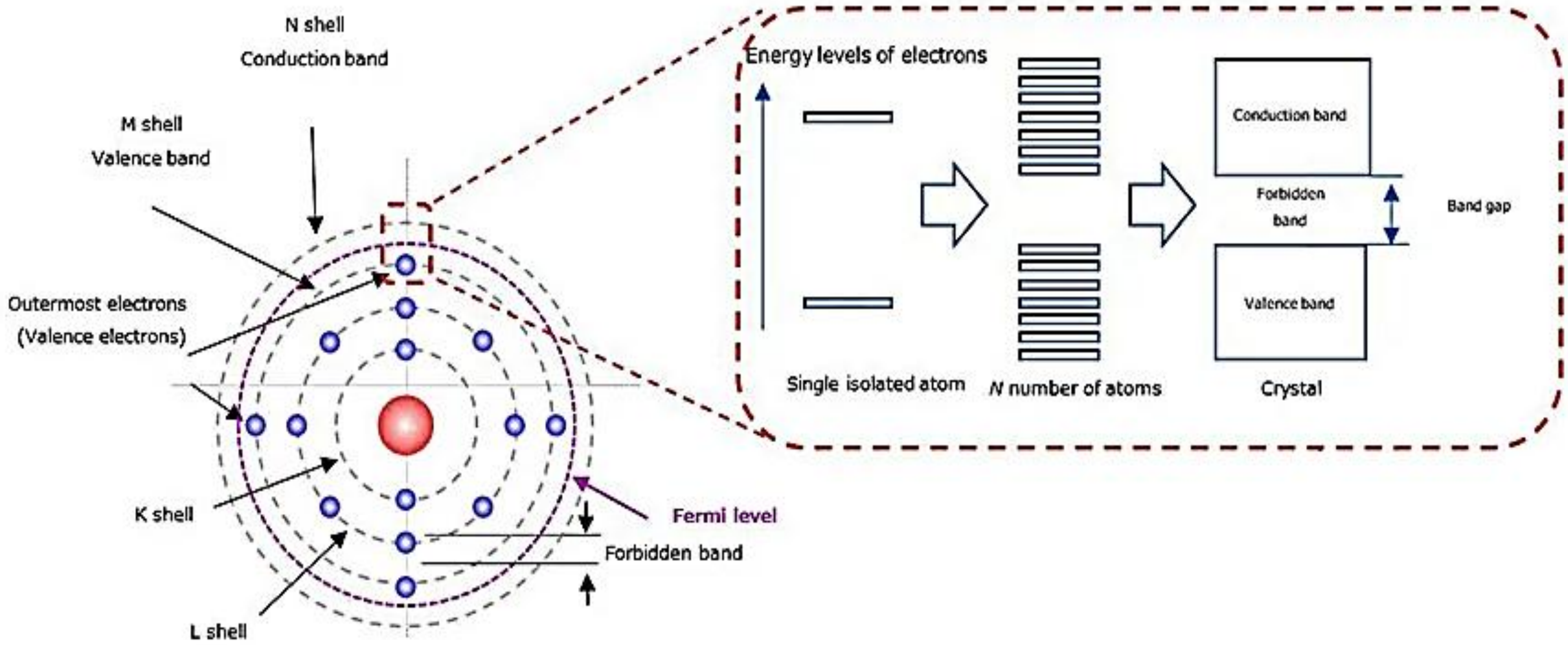
Energy Bands in Solids

- According to Quantum Mechanical Laws, the energies of electrons in a free atom can not have arbitrary values but only some definite (quantized) values.
- However, if an atom belongs to a crystal, then the energy levels are modified.
- This modification is not appreciable in the case of the inner shells (completely filled).
- But in the outermost shells, modification is appreciable because the electrons are shared by many neighboring atoms.
- Due to influence of high electric field between the core of the atoms and the shared electrons, energy levels are split-up or spreadout forming energy bands.



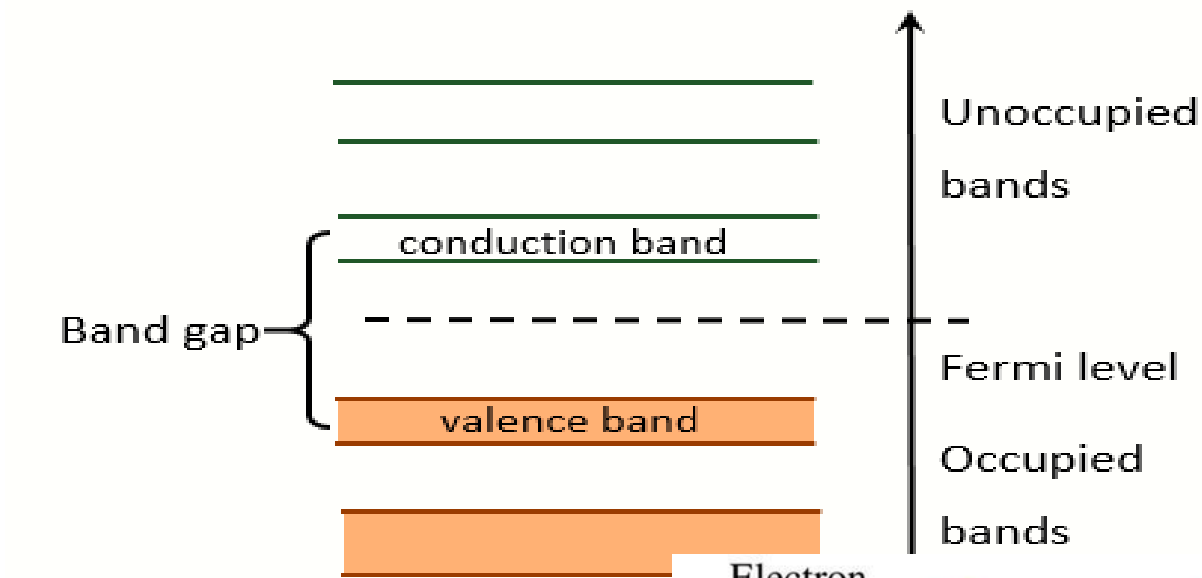
Formation of Energy Bands in Solids

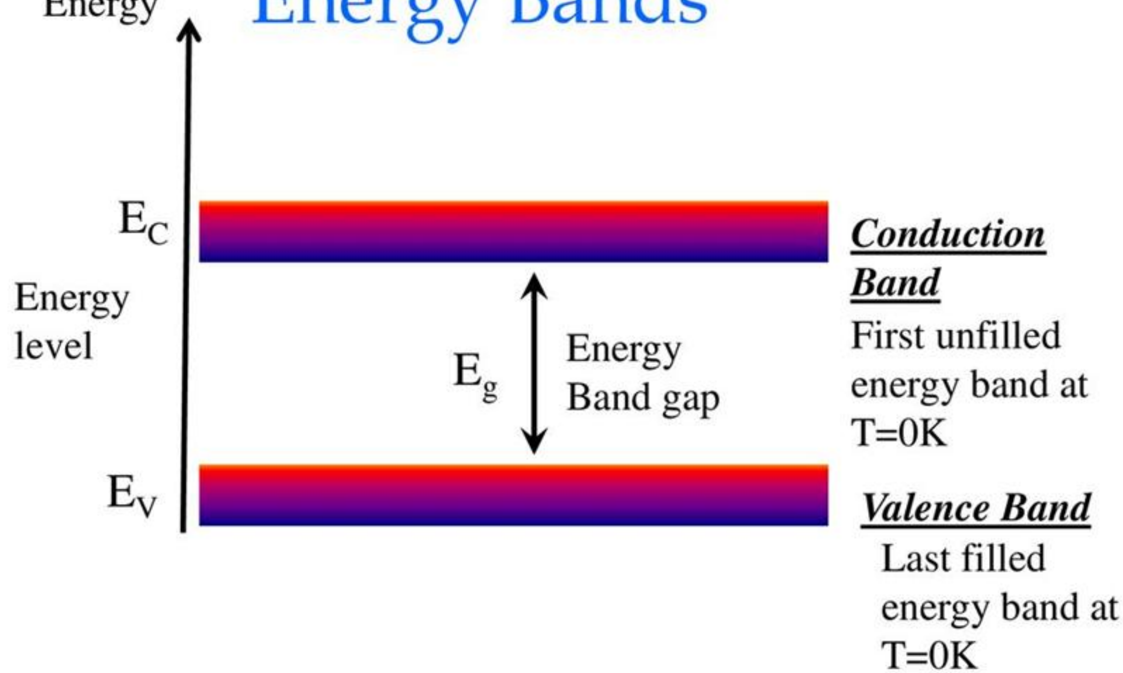


The highest energy level occupied by electrons in the conduction band in a crystal, at absolute zero temperature, is called **Fermi Level.**

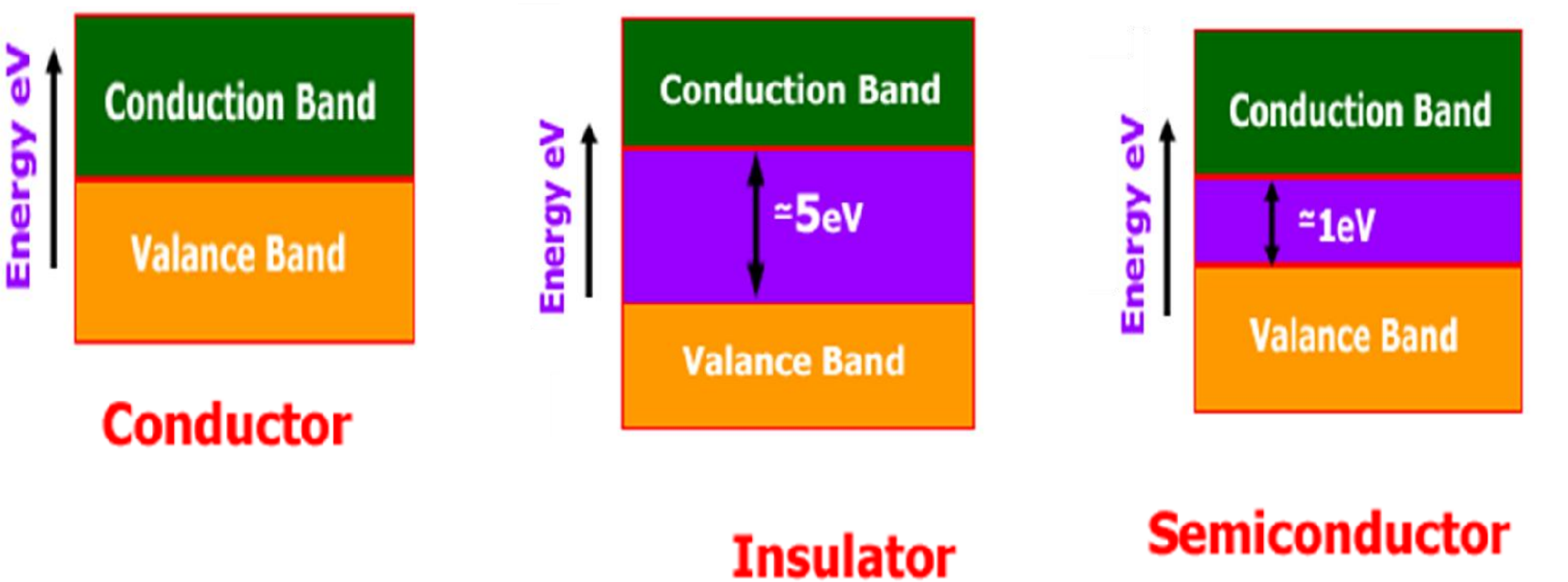
The energy corresponding to this energy level is called **Fermi energy** (E_f).

Energy Bands





Classification of solids based on Energy Band gap

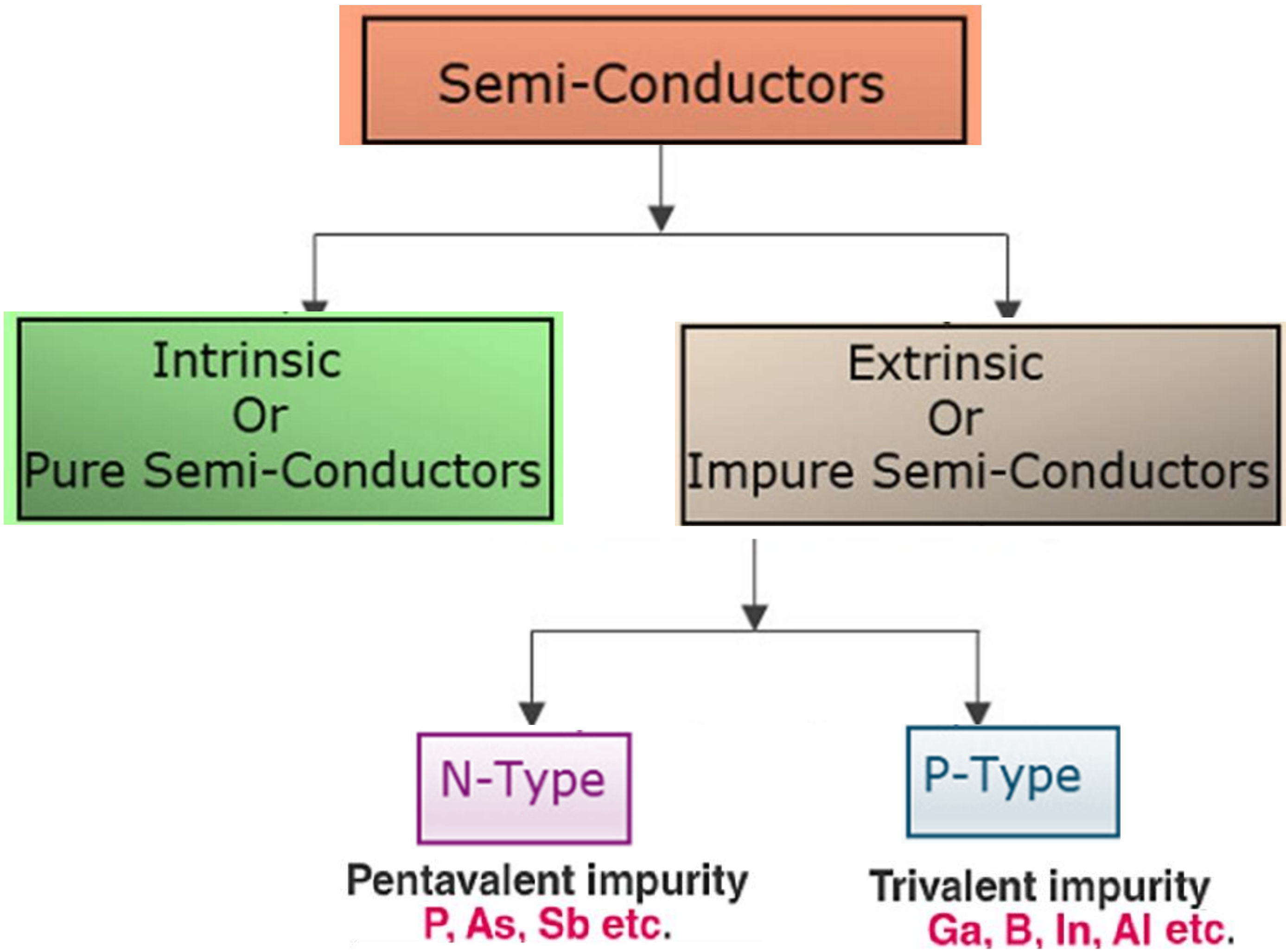


Semiconductors

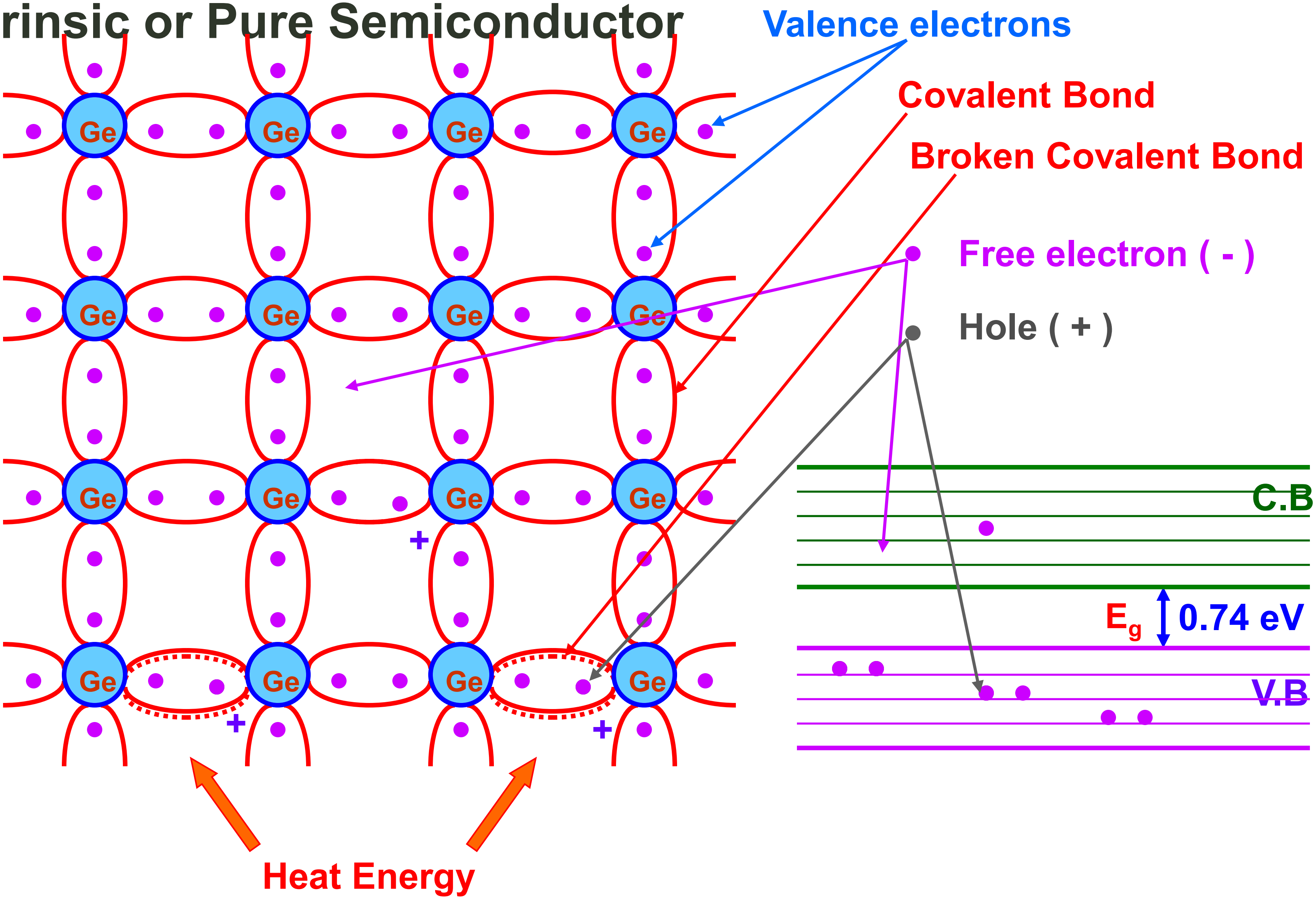
- **Semiconductors are materials having energy band gap in between conductors and insulators (approximately 1eV)**

- **They have conductivity between conductors (generally metals) and nonconductors or insulators (such as most ceramics).**
- **Resistivity:** 10^{-5} to 10^{6} Ωm, **Conductivity:** 10^{5} to 10^{-6} mho/m
- **Temperature coefficient of resistance:** Negative
- **Current flow:** Due to electrons and holes

- **Semiconductors can be pure elements, such as silicon or germanium, or compounds such as gallium arsenide or cadmium selenide.**


Semi-Conductors
Intrinsic
Or
Pure Semi-Conductors
Extrinsic
Or
Impure Semi-Conductors
N-Type
Pentavalent impurity
P, As, Sb etc.
P-Type
Trivalent impurity
Ga, B, In, Al etc.

Intrinsic or Pure Semiconductor



If n and p represent the electron and hole concentrations respectively then

$$\boxed{(n)\,(p) = (n_i)(p_i) = n_i^2}$$

where n_i and p_i are the intrinsic carrier concentrations.

Drawbacks of intrinsic or pure semiconductors

- A room temperature, it has a very small number of current carriers (electrons and holes).
- Hence, its conductivity is low.
- Dependence on temperature only

DOPING IN SEMICONDUCTORS

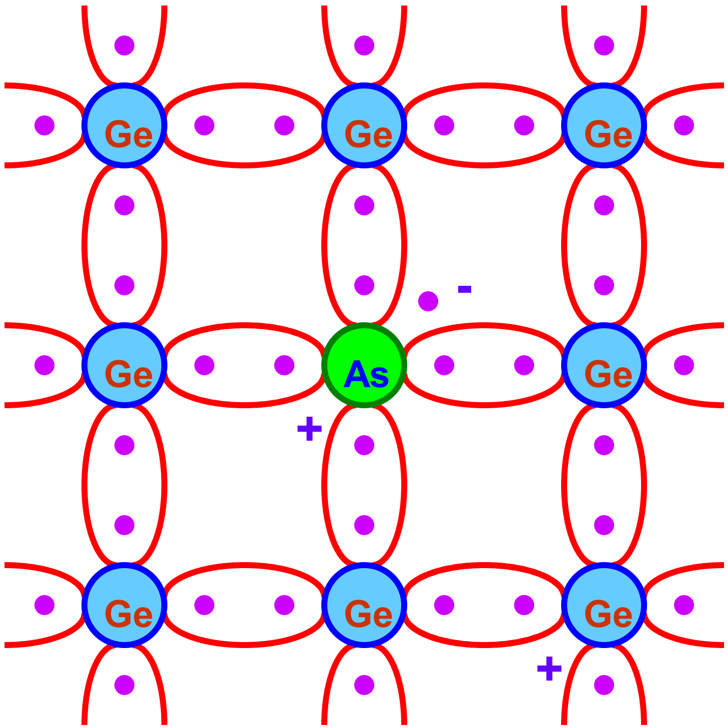
- Semiconducting materials are very sensitive to impurities in the crystal lattice.
- The controlled addition of these impurities into pure semiconductor is known as **doping.**
- Allows the tuning of the electronic properties: technological applications.
- Introduction of dopants →'extrinsic semiconductors'.

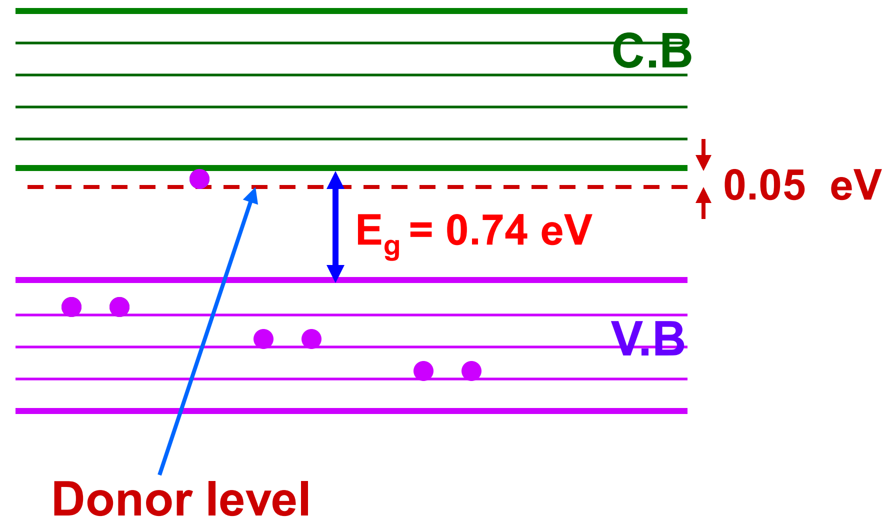
  (a) Increase in the conductivity

  (b) New intra-band, energy levels

  (c) Generation of positive or negative charge carriers.

N - Type Semiconductors





When a semiconductor such as Si or Ge is doped with a pentavalent impurity (Group V elements such as P, As or Sb), N – type semiconductor is formed.

When germanium (Ge) is doped with arsenic (As), the four valence electrons of As form covalent bonds with four Ge atoms and the fifth electron of As atom is loosely bound.

- The energy required to detach the fifth loosely bound electron is only of the order of 0.05 eV for germanium.

- Therefore, the energy state corresponding to the fifth electron is in the forbidden gap and slightly below the lower level of the conduction band.

- This energy level is called ‘donor level’. The impurity atom is called ‘donor’.

- N – type semiconductor is called ‘donor – type semiconductor’.

- When intrinsic semiconductor is doped with donor impurities, not only does the number of electrons increase, but also the number of holes decreases.

- Therefore, in an N-type semiconductor, free electrons are the majority charge carriers and holes are the minority charge

❖ If n and p represent the electron and hole concentrations respectively then

$$\boxed{(n)\,(p) = n_i^{\,2}}$$

Where, n_i and p_i are the intrinsic carrier concentrations.

❖ For N type material at room temperature

$$(n_n)\,(p_n) = n_i^{\,2}$$

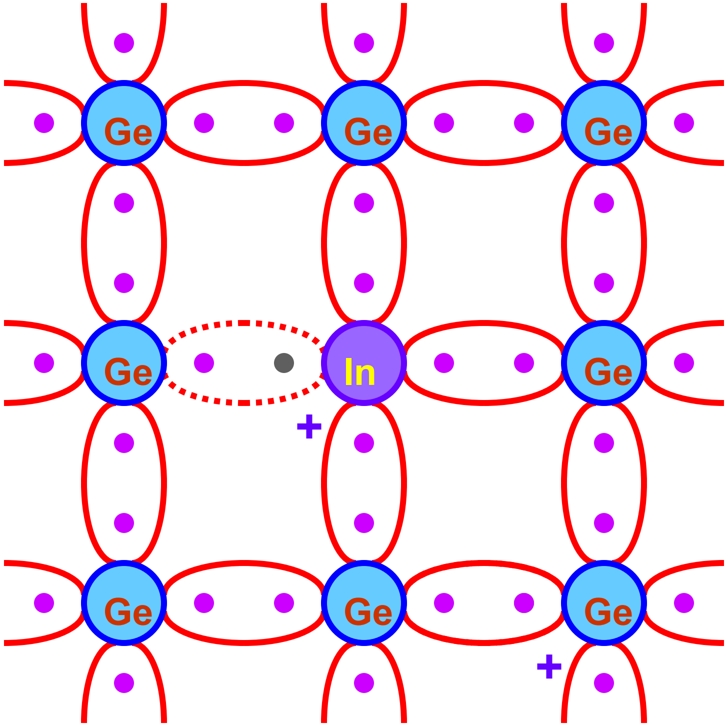
❖ Let N_D is the number of donors per unit volume.

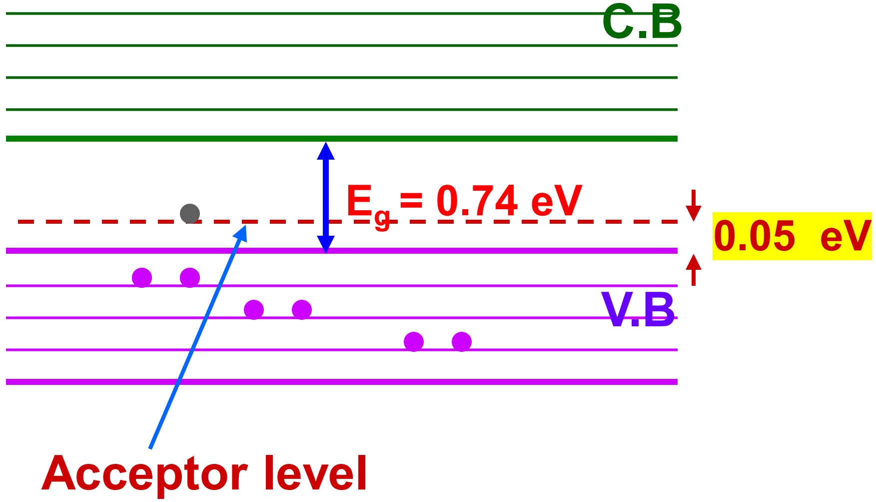
Majority carrier concentration $n_n \approx N_D$

$$(N_D)\,(p_n) = n_i^{\,2}$$

Minority carrier concentration $p_n \approx \dfrac{n_i^{\,2}}{(N_D)}$

P - Type Semiconductors





When a semiconductor such as Si or Ge is doped with a trivalent impurity (Group III elements such as In, B or Ga), P – type semiconductor is formed.

After doping, the three valence electrons of impurity form three covalent bonds with three Ge atoms. The vacancy that exists with the fourth covalent bond constitutes a **hole.**

- The hole may be filled with an electron from neighboring atom, creating a hole in that position from where the electron jumped.
- Therefore, the trivalent impurity atom is called **'acceptor'.**
- Since the hole is associated with a positive charge moving from one position to another, therefore, this type of semiconductor is called **P – type semiconductor.**
- The acceptor impurity produces an energy level just above the valence band known as **'acceptor level'.**
- P – type semiconductor is called **'acceptor – type semiconductor'.**
- In a P – type semiconductor, holes are the majority charge carriers and the electrons are the minority charge carriers.

- If n and p represent the electron and hole concentrations respectively then $\boxed{(n)\,(p) = n_i^{\,2}}$

where n_i and p_i are the intrinsic carrier concentrations.

- For P type material at room temperature

$$(n_p)\,(p_p) = n_i^{\,2}$$

Let N_A is the number of acceptors per unit volume.

Majority carrier concentration $p_p \approx N_A$

$$(n_p)\,(N_A) = n_i^{\,2}$$

Minority carrier concentration $n_p \approx \dfrac{n_i^{\,2}}{(N_A)}$

Important Formulae and Concepts related to Conductor

1. Drift Velocity
2. Mobility
3. Current and Current Density
4. Resistance and Resistivity
5. Microscopic Ohm's Law
6. Expression for Conductivity and Resistivity

Refer Class Notes

Conductivity in intrinsic Semiconductor

- The conductivity of conductor is given by $\sigma = (n)(e)(\mu)$

- For semiconductor, the conductivity will be due to n type and p type

$$\sigma = (\sigma_n) + (\sigma_p)$$

$$\sigma = (n)(e)(\mu_n) + (p)(e)(\mu_p)$$

μ_n and μ_p refer to the mobilities of the electrons and holes *n* and *p* refer to the density (concentration) of electrons and holes respectively.

For intrinsic semiconductors n = p = n_i (intrinsic charge carrier density)

$$\sigma = (n_i)(e)(\mu_n) + (n_i)(e)(\mu_p)$$

$$\boxed{\sigma = (n_i)(e)(\mu_n + \mu_p)}$$

Conductivity in Extrinsic Semiconductor

- In doped semiconductor (Extrinsic), majority carriers greatly out numbers the minority carriers, so that the equation can be reduced to a single term involving the majority carrier.

- For n-type semiconductor, $\sigma_n = (n)(e)(\mu_n)$

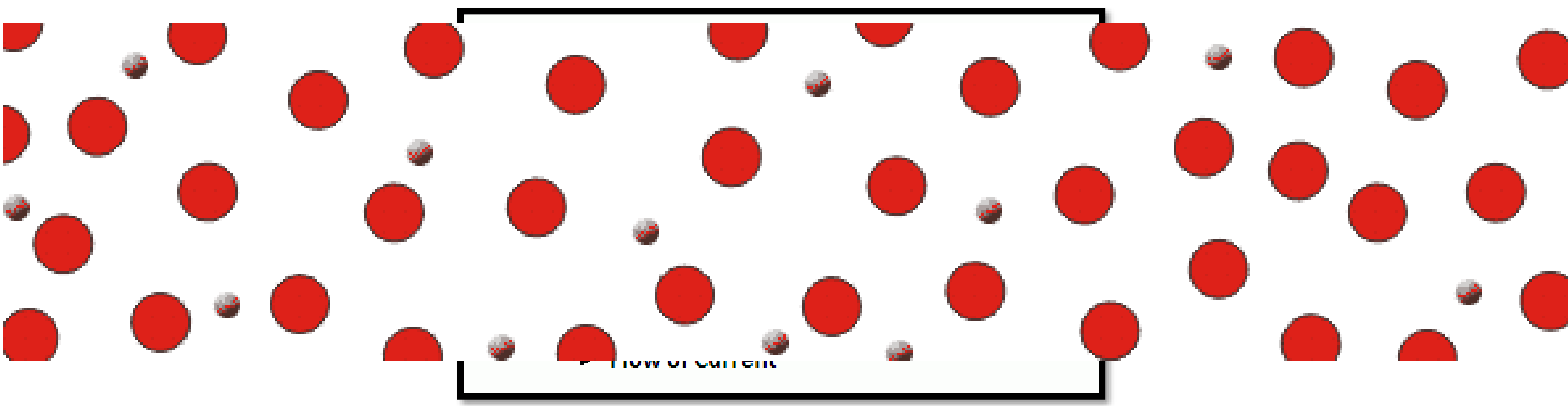
- For p-type semiconductor, $\sigma_p = (p)(e)(\mu_p)$

- Conductivity of a material is determined by two factors:
  (i) concentration of free carriers available to conduct current
  (ii) their mobility (or freedom to move).

In a semiconductor, both mobility and carrier concentration are temperature dependent.

Drift current

- Absence of field: free electrons and holes move with random velocities and random directions.
- Presence of field: the randomly moving electrons and holes experience an electrical force.
- Electrons shift towards higher potential and holes towards lower potential.



https://web2.ph.utexas.edu/~coker2/index.files/current.htm

- The drift movement of electrons and holes inside an electrically stressed conductor, is known as drift current.
- The drift current density for electron and hole are given by

$$J_{(drift)electron} = -(n)(e)(\mu_n)(E)$$

$$J_{(drift)hole} = (p)(e)(\mu_p)(E)$$

- where n, p are the electron and hole densities, μ_n and μ_p are mobility of electron and holes respectively.
- Negative sign indicates that the electrons having -ve charge move in direction opposite to the applied field.
- Total drift current density

$$J_{(drift)Total} = J_{(drift)electron} + J_{(drift)hole}$$

The drift current density for electron and hole are given by

$$J_{(drift)electron} = -(n)(e)(\mu_n)(E)$$

$$J_{(drift)hole} = (p)(e)(\mu_p)(E)$$

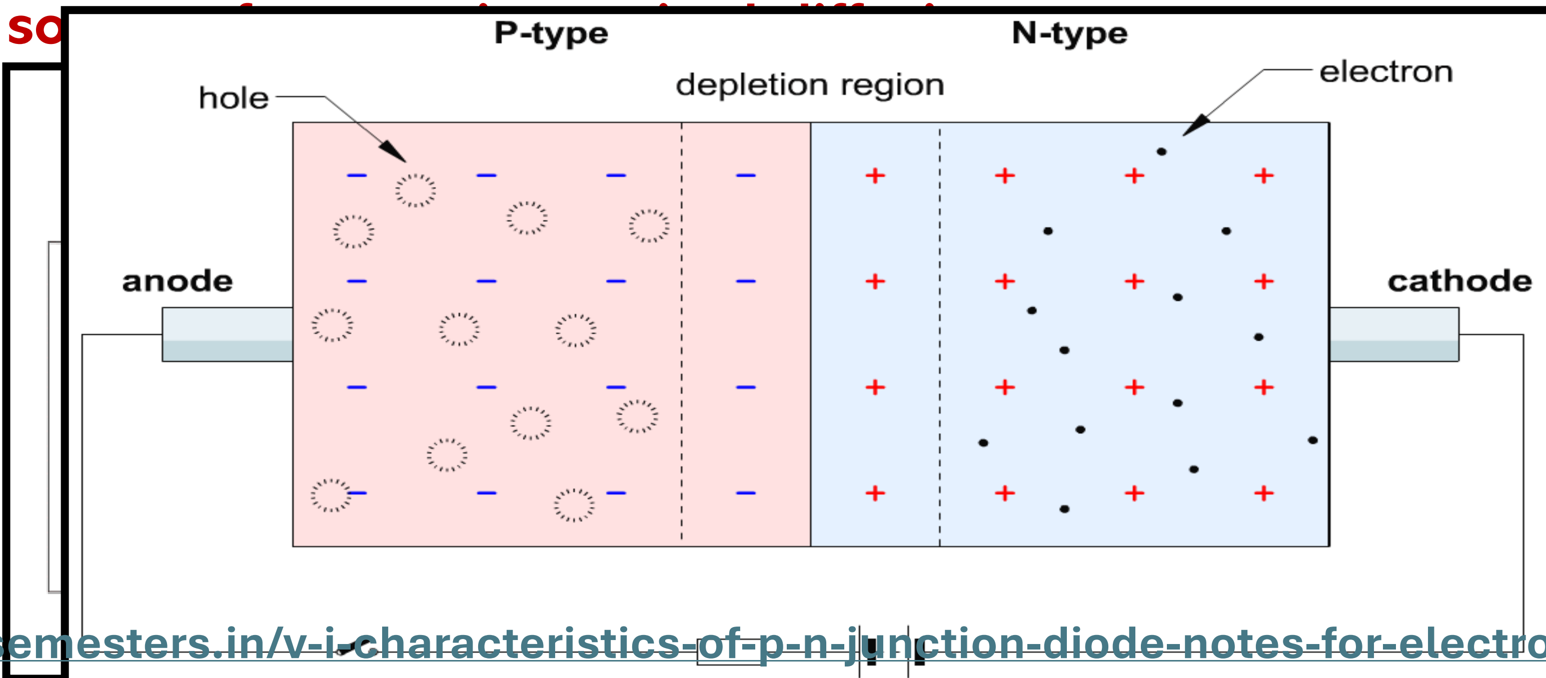
Total drift current density

$$J_{(drift)Total} = J_{(drift)electron} + J_{(drift)hole}$$

$$J_{(drift)Total} = -(n)(e)(\mu_n)(E) + (p)(e)(\mu_p)(E)$$

Diffusion current

- In semiconducting material → Dopants are introduced to some region → even distribution of carriers takes place to maintain the uniformity
  → known as diffusion process
- Movement of the mobile charge carriers are responsible for the flow of diffusion current from one region to the other.
- No so



http://semesters.in/v-i-characteristics-of-p-n-junction-diode-notes-for-electronics-eng

- Non-uniformity of charge carriers (electrons/holes) → gives the diffusion current (is independent of the electric field) → depends on the concentration gradient.
- Concentration of electrons (*n*) and holes (*p*) varies with the distance *x*.
- Diffusion current density for electrons $J_{(diff)electron} = (e)(D_n)(\frac{dn}{dx})$, where D_n is the diffusion coefficient for electrons and (dn/dx) is the concentration gradient of electrons.
- Diffusion current density for holes $J_{(diff)hole} = -(e)(D_p)(\frac{dp}{dx})$, where D_p is the diffusion coefficient for holes and (dp/dx) is the concentration gradient of holes.
- Resultant diffusion current density for both holes and electrons is given as $J_{(diff)Total} = J_{(diff)electron} + J_{(diff)hole}$

$$J_{(diff)Total} = (e)(D_n)(\frac{dn}{dx}) - (e)(D_p)(\frac{dp}{dx})$$

Total current density in semiconductor is the sum of drift current and diffusion current is given by

$$J_{Total} = J_{drift} + J_{diffusion}$$

$$J_{Total} = J_{(drift)electron} + J_{(drift)hole} + J_{(diffusion)electron} + J_{(diffusion)hole}$$

$$J_{Total} = -(\mathbf{n})(e)(\mu_n)(\mathbf{E}) + (\mathbf{p})(e)(\mu_p)(\mathbf{E}) + (e)(D_n)\left(\frac{dn}{dx}\right) - (e)(D_p)\left(\frac{dp}{dx}\right)$$

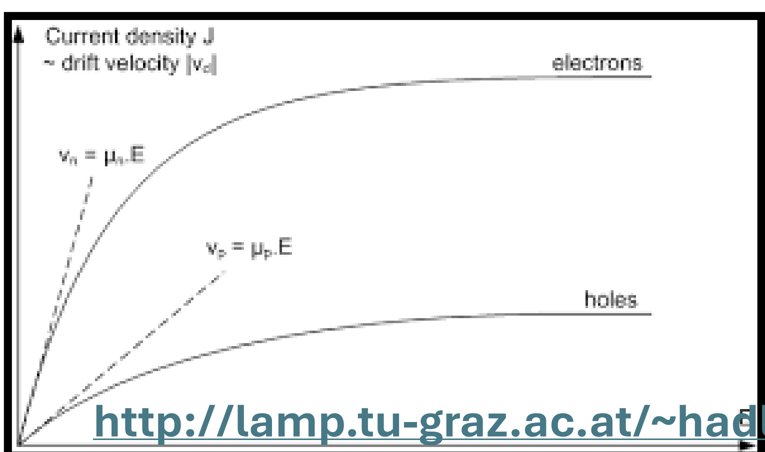


Figure shows the plot for the current density J_{drift} and the absolute value of the drift velocity, over the electric field E. The mobility of holes and electrons can be evaluated using the tangential of the drift velocity.

http://lamp.tu-graz.ac.at/~hadley/psd/problems/diffusioncurrent2/s.pdf

Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics

- When system consists of several energy levels (and each energy level could also have several energy states) then concept of statistics is needed.
- A particle in this system can be in one of those energy levels depending on the energy particle has. It is impossible to have just one particle in a system since in real life it needs various particles to constitute a system. They occupy the levels under a statistics rule.
- **There are three statistics:**

1. **Maxwell Boltzmann statistics** is applicable to identical, distinguishable particle of any type spin. The molecules of gas are particle of this type.
2. **Bose Einstein statistics** is applicable to the identical, indistinguishable particles of zero or integral spin. These particles are called Bosons. Example photons, Helium atom
3. **Fermi Dirac statistics** is applicable to the identical, indistinguishable particles of half-integral spin. These particles obey Pauli Exclusion Principle. Example Electron, proton etc.

Maxwell-Boltzmann	Bose-Einstein	Fermi-Dirac
*Particles are identical and distinguishable	*Their Particles are indistinguishable	*Their particles are indistinguishable
*The number of particles is constant	*Particles do not obey Pauli exclusion principle	*Particles obey Pauli exclusion principle
*The total Energy is constant	*Each state can have more than one particle like phonons and photons	*Each state can have only one particle
*Spin is ignored	*Particles have integer spin	*Each particle has one half spin

Fermi Dirac distribution function

- The probability density functions describes the probability that particles occupy the available energy levels in a given system.

- Fermions : half-integer spin particles - Electrons are Fermions- obeys Pauli exclusion principle → one Fermion occupies a single quantum state → fills the available states in an energy band.

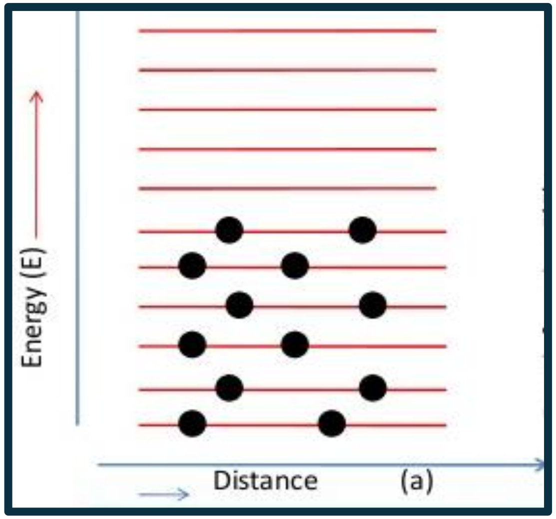
- Fermi function : The probability that an energy level at energy, *E* in thermal equilibrium with a large system, is occupied by an electron.

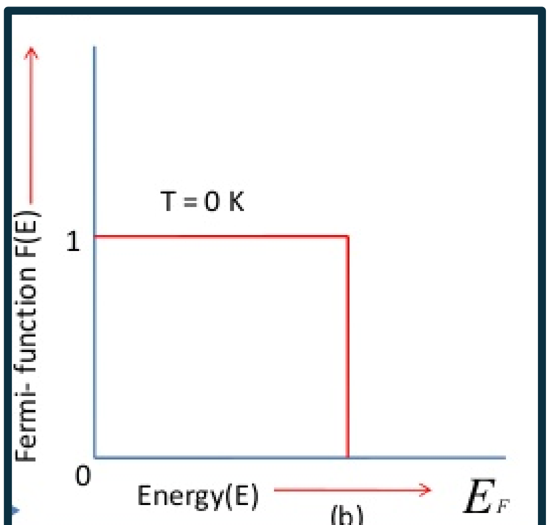
- Fermi Dirac distribution function is given as:

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

E_F : Fermi energy; k : Boltzmann constant; T: Temperature

FERMI LEVEL IN A CONDUCTOR





Fermi function is $f(E) = \frac{1}{1+e^{(E-E_F)/kT}}$

Case 1: At T= 0 K; E< E_F => (E-E_F) is negative

$\therefore f(E) = \frac{1}{1+e^{-(E-E_F)/0}} = \frac{1}{1+e^{-\infty}} = \frac{1}{1+0} = 1$

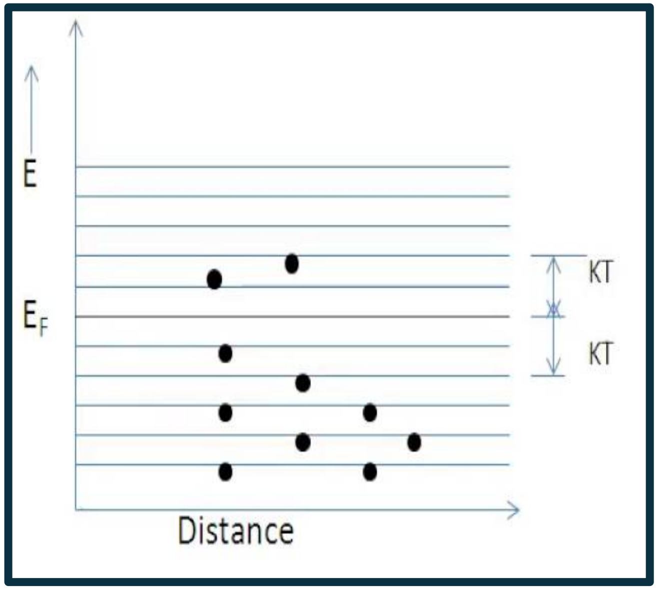
All *levels lying below* E_F are occupied.

Case 2: At T= 0 K; E> E_F => (E-E_F) is positive

$\therefore f(E) = \frac{1}{1+e^{(E-E_F)/0}} = \frac{1}{1+e^{\infty}} = \frac{1}{1+\infty} = \frac{1}{\infty} = 0$

All energy levels lying above E_F are vacant

What happens to the fermi level at high temperature ?

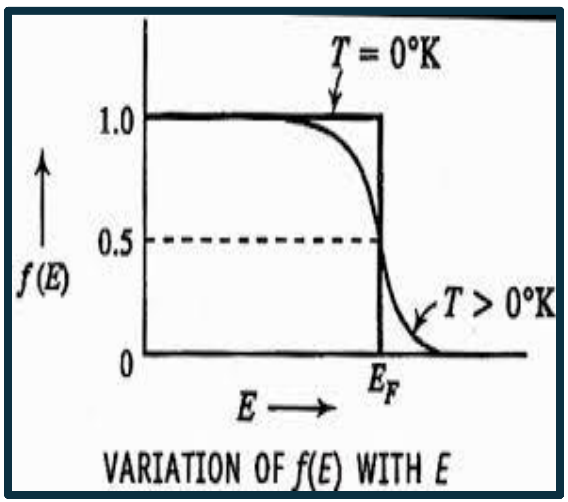


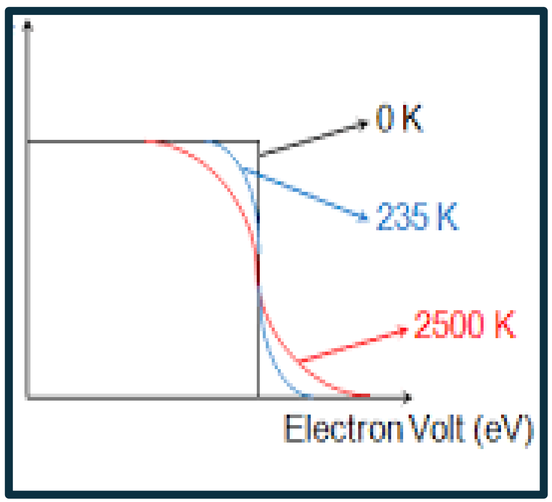
Case 3: At T > 0 K; E = E_F

$$\therefore f(E) = \frac{1}{1+e^{\left(\frac{0}{kT}\right)}} = \frac{1}{1+e^{0}} = \frac{1}{1+1} = \frac{1}{2}$$

The probability of occupancy at any temperature T > 0 K is 50 %.

<u>Fermi energy</u>: Average energy possessed by electrons participating in conduction at temperature above 0K.





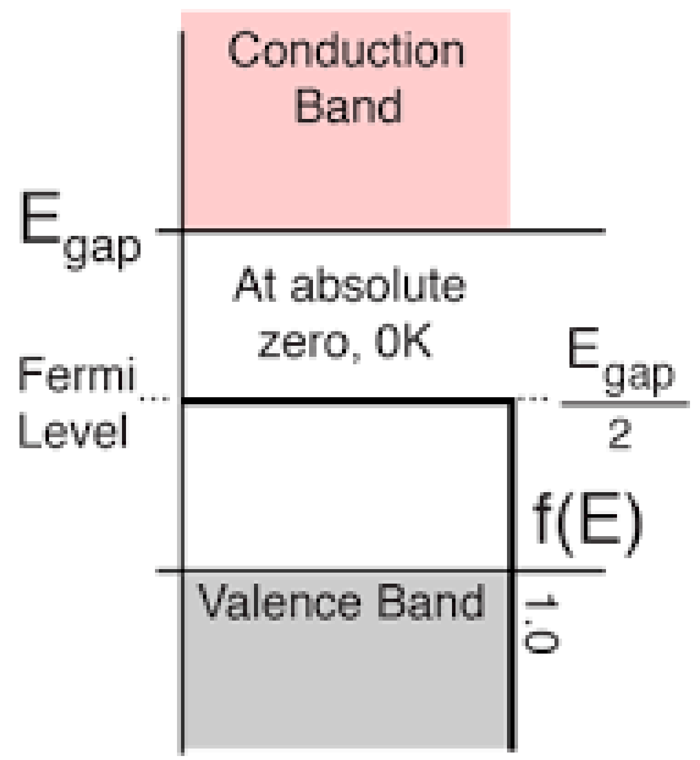
***<u>Fermi velocity: v_F</u>*: It is the velocity of the electrons in the highest occupied states in metals at zero temperature.**

$$v_F = \sqrt{2E_F/m}$$

https://www.electrical4u.com/fermi-dirac-distribution-function/

What is fermi level ?

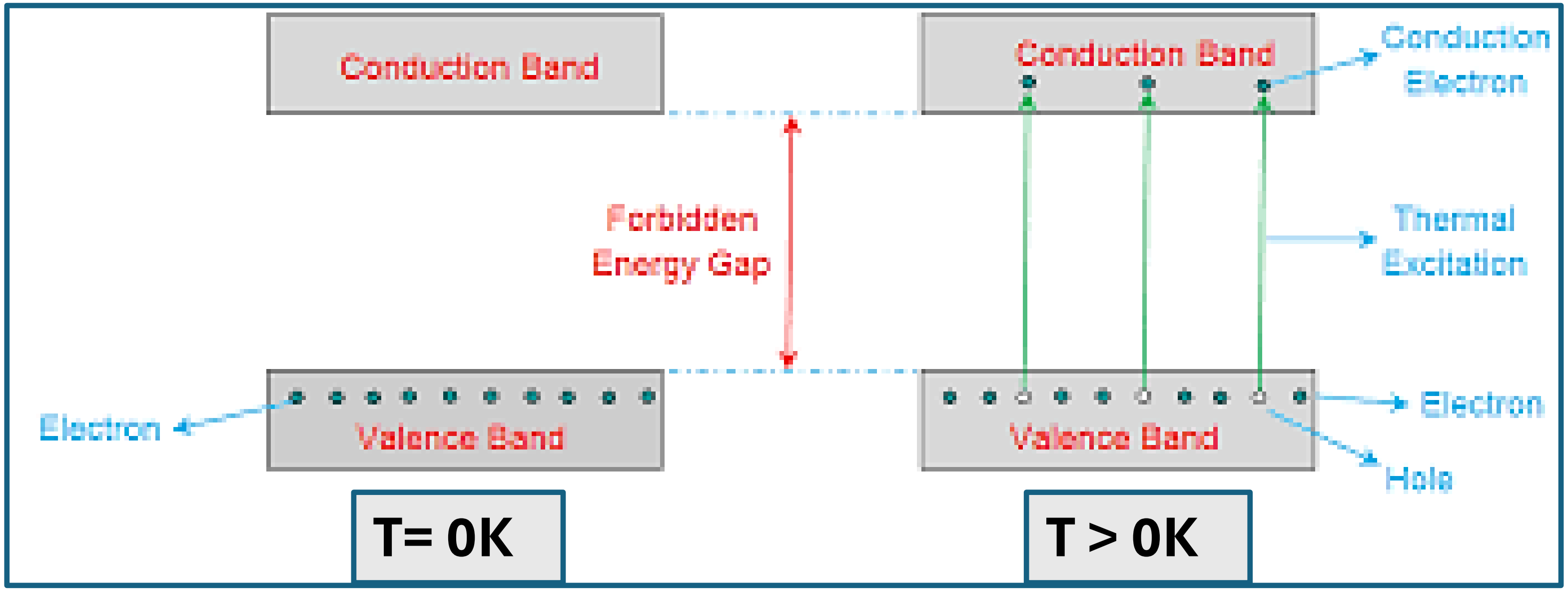
- The highest energy level that an electron occupies at the absolute zero temperature is known as the Fermi Level.
- The Fermi level lies between the valence band and conduction band. At T=0 K, the electrons are all in the lowest energy state → Fermi level can be considered as the sea of fermions (or electrons) above which no electrons exist.
- The Fermi level changes as the temperature increases or electrons are added to or withdrawn from the solids.



Context of Fermi level for a semiconductor

Fermi level in intrinsic semiconductor

- At T = 0 K, the valence band will be full of electrons → impossible to cross the energy barrier → acts as an insulator.
- At T > 0 K → the electron movement from the valence band to the conduction band increases → create holes in the valence band in place of electrons.
- The electron concentration '*n*' is equal to hole concentration '*p*'.



Position of Fermi level in intrinsic semiconductor

Let, n be the number of electrons in the semiconductor band and p be the number of holes in the valence band.

At temperature T > 0 K

$$n = N_c e^{-(E_c - E_F)/kT} \qquad p = N_v e^{-(E_F - E_V)/kT}$$

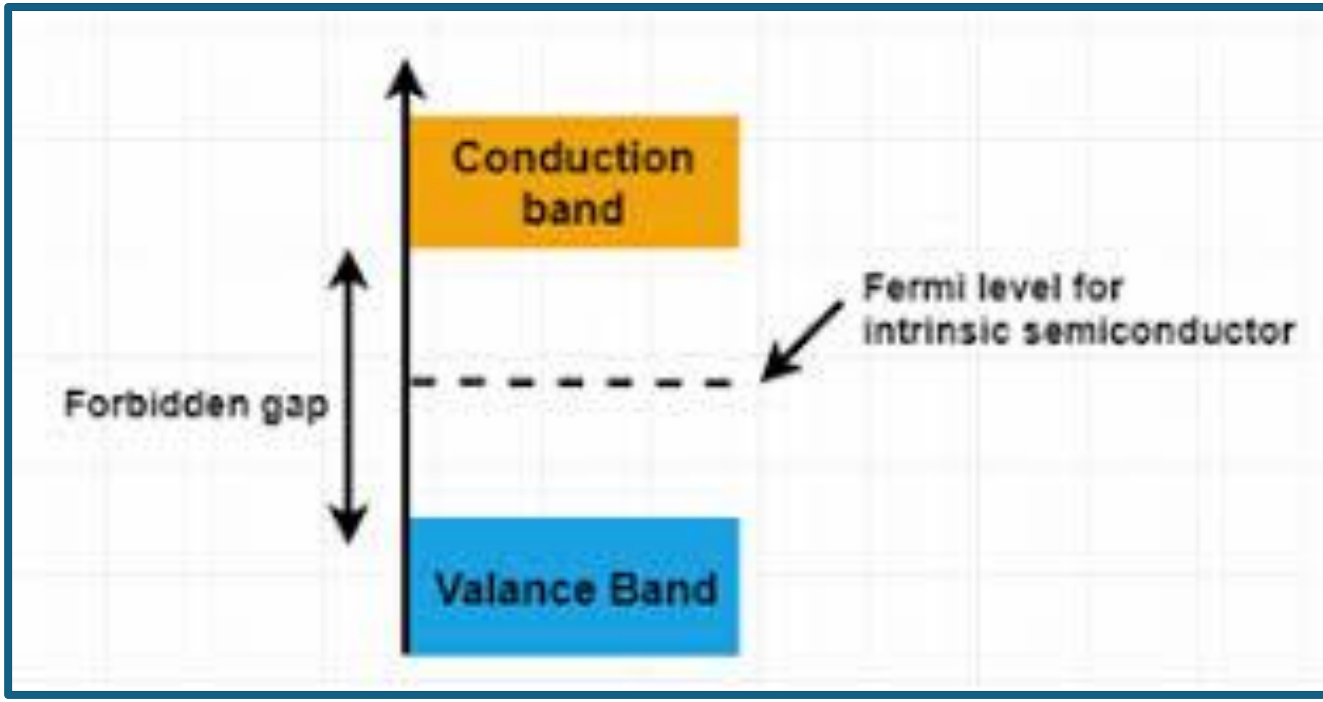
N_c is the effective density of states in the conduction band and N_v is the effective density of states in the valence band. For an intrinsic semiconductor, $n_e = n_v$

$$N_c e^{-(E_c - E_F)/kT} = N_v e^{-(E_F - E_v)/kT} \Rightarrow \frac{N_C}{N_v} = \frac{e^{-(E_F - E_V)/kT}}{e^{-(E_c - E_F)/kT}}$$

$$\Rightarrow e^{\frac{-(2E_F - E_V - E_C)}{kT}} = 1 \text{ as } N_c = N_v$$

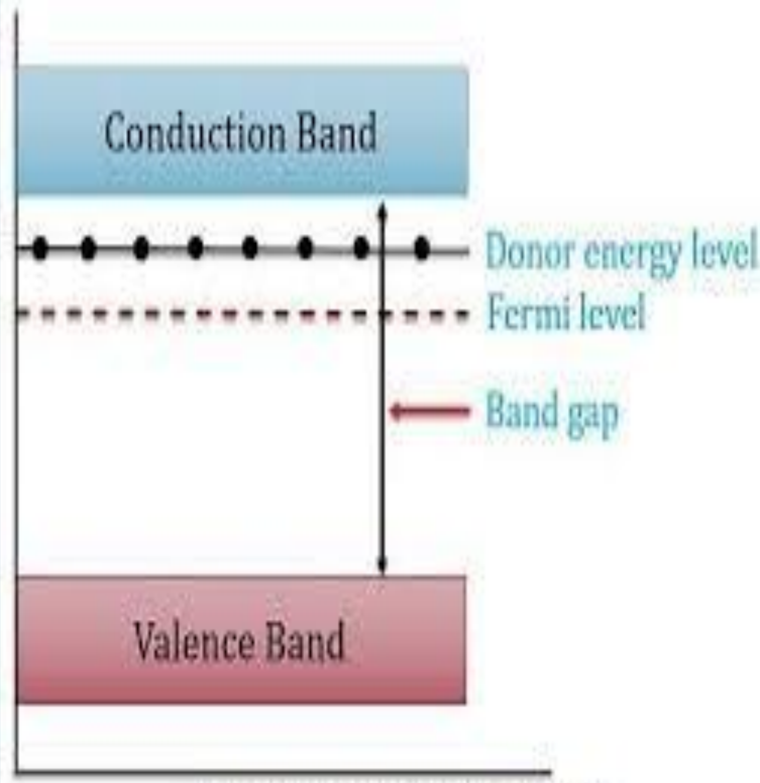
Taking log on both sides, we get $\frac{E_c + E_v - 2E_F}{kT} = 0 \Rightarrow \boxed{E_F = \frac{E_C + E_V}{2}}$

∴ Fermi level in an intrinsic SC → at the centre of the band gap.

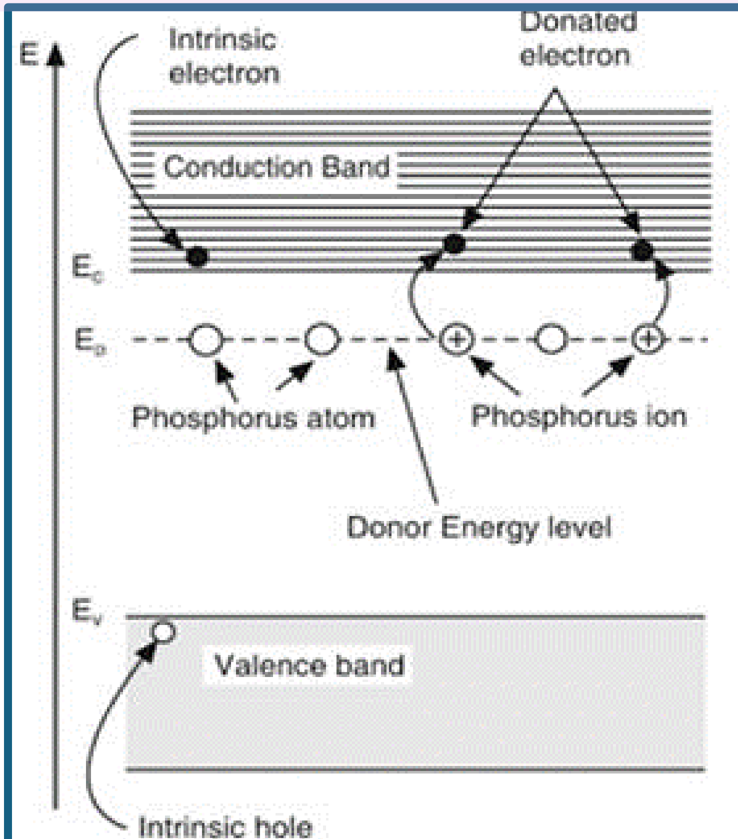

Conduction band
Fermi level for intrinsic semiconductor
Forbidden gap
Valance Band

Fermi level in N-type semiconductor

In n-type SC- pentavalent impurity : electrons as majority charge carriers: donor impurities



Energy level diagram of N type semiconductor

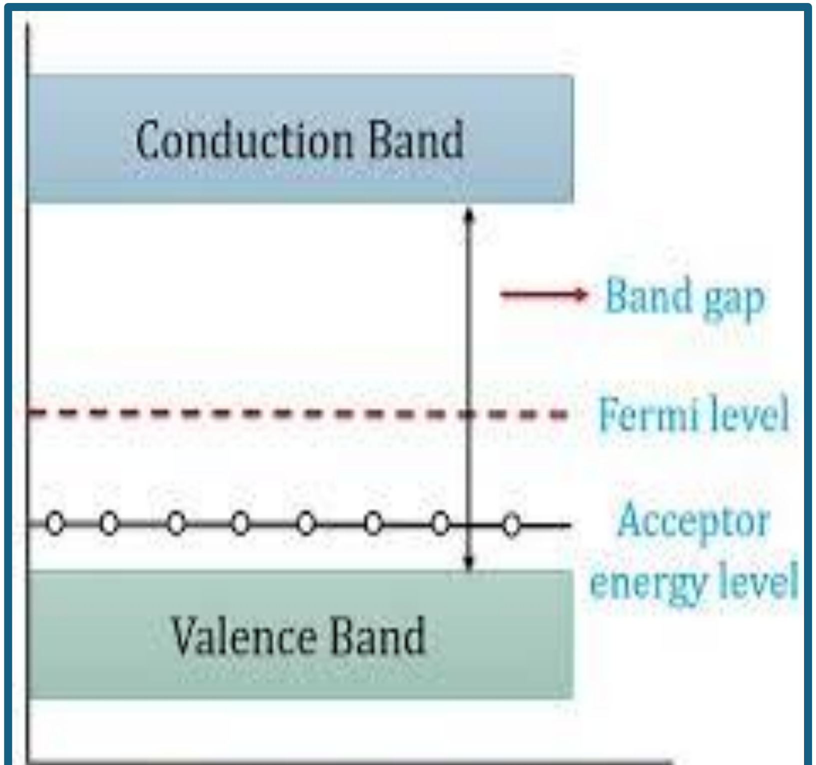


: Energy band diagram of n-type semiconductor

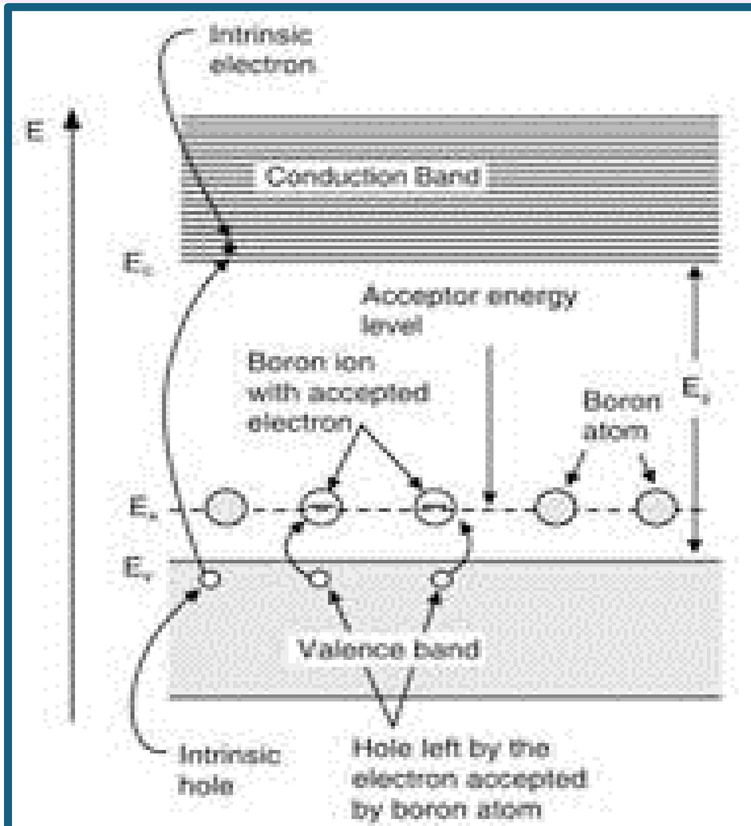
https://sites.google.com/site/puenggphysics/home/unit-5/fermi-level-of-extrinsic-semiconductor

Fermi level in P-type semiconductor

In p-type SC- trivalent impurity : holes as majority charge carriers known as acceptor impurities



Energy level diagram of P type semiconductor



Energy band diagram for a p-type semiconductor

https://sites.google.com/site/puenggphysics/home/unit-5/fermi-level-of-extrinsic-semiconductor