Functional Properties

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Introduction

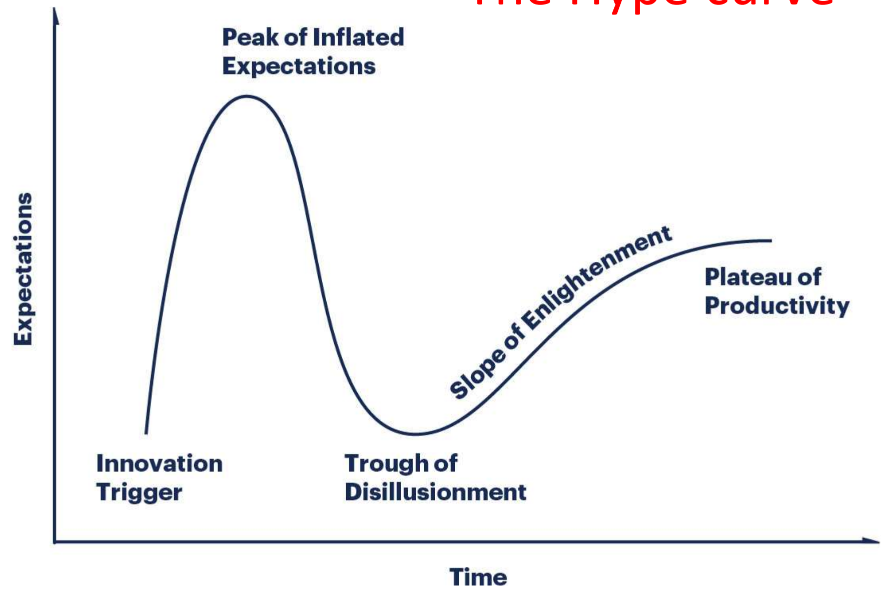
- Technology has enabled many marvels
- Smart phones help patients connect with their near and dear ones
- Our classes are running on smart phone. Devices are everywhere
- Remote medicine and surgery to making Mangalyan and Chandrayan possible
- Alexa was like science fiction to someone like me
- These days kids use it to solve their homework

- Electricity led to industrial revolution
- Gas tubes and later semiconductors led to computing
- Magnetic memory size has reduced
- Floppy to CD to DVD to USB
- My cheap smart phone today is better than the first desktop my father bought for me in 2000
- Industry 4.0 the next industrial revolution
- Cyber physical world

- Internet of things is in our homes
- Many equipment employ artificial intelligence algorithms
- More machines so are we loosing humanity
- Affective computing
- Can we predict depression in an individual without him/her seeing a doctor
- Invasion in your privacy
- We are at the fringe of ethical territory hence, social sciences important

- ➢ Fortunately or unfortunately we do not have to worry about this in the present course
- ➢ But should we never worry at all
- ➢ Reading science fiction and even novels and novella on your tab
- ➢ For what you may think as fiction today may become reality in your lifetime

The Hype curve



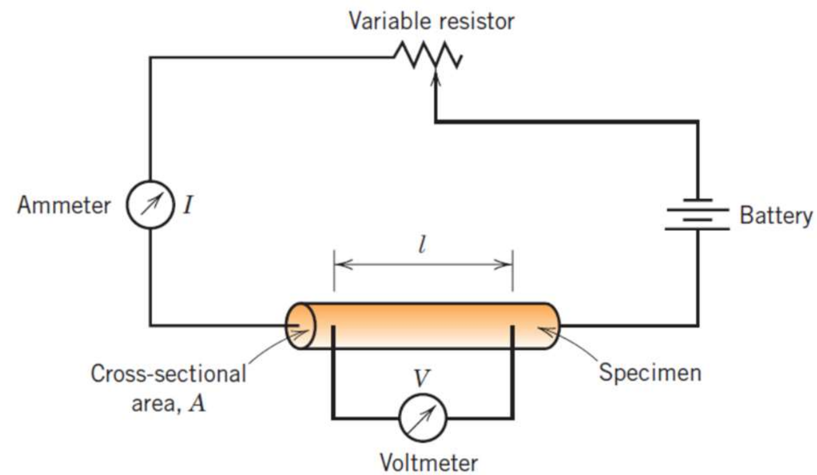
You must dream to change the world not to find a job that gives you enough money to enjoy the night life in your favourite city !

Electrical conduction

- Ohm's law

- Electrical resistance and resistivity

- Electrical conductivity



Current per unit area or current density J
Voltage per unit length is electric field intensity,

$$V = IR$$

$$\rho = \frac{VA}{Il}$$

$$\rho = \frac{RA}{l}$$

$$\sigma = \frac{1}{\rho}$$

$$J = \sigma \mathscr{E}$$

$$\mathscr{E} = \frac{V}{l}$$

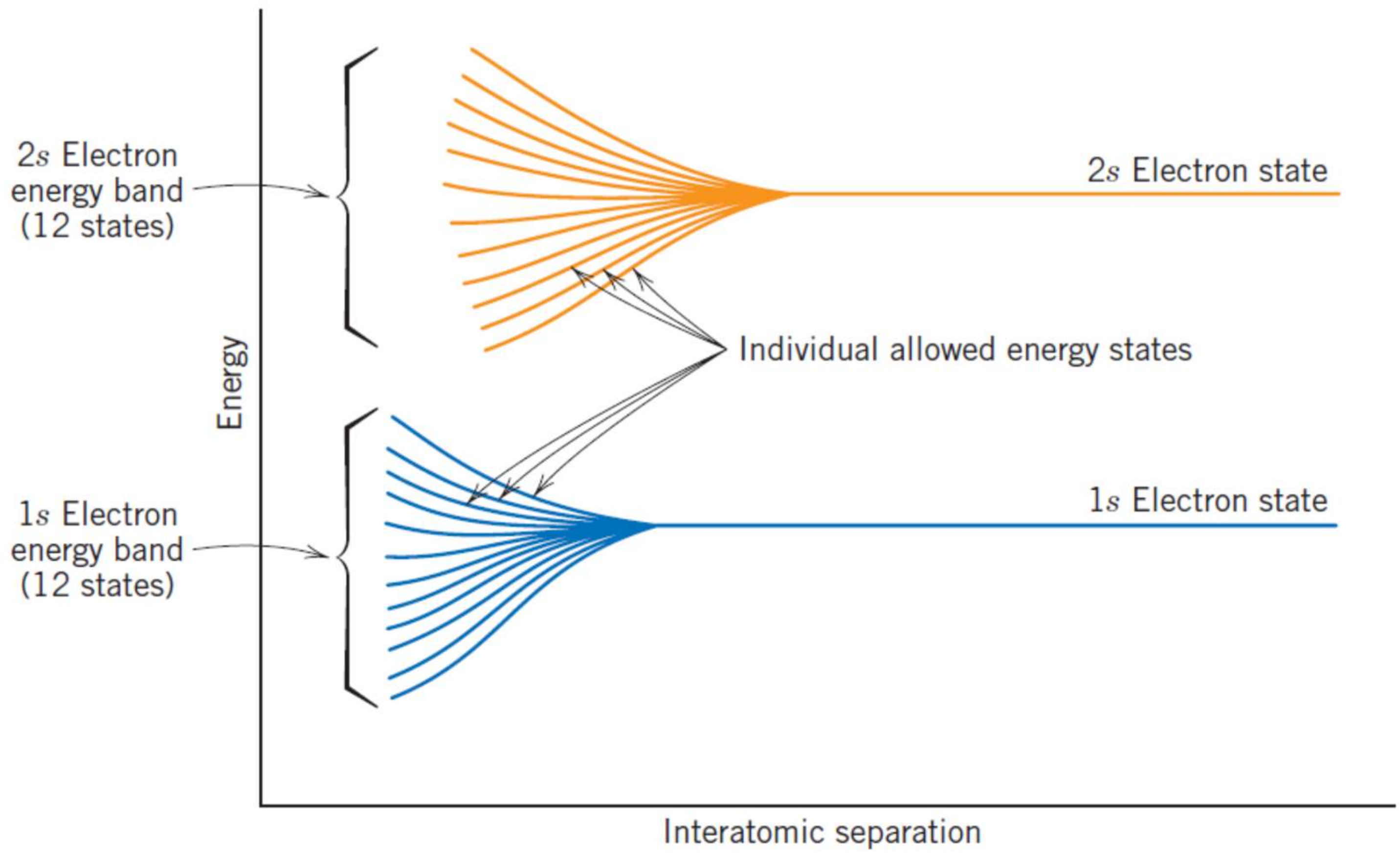
- Current in Ampere, voltage in volts and resistance in Ohm
- Ohm the SI unit of electrical resistance, transmitting a current of one ampere when subjected to a potential difference of one volt
- Inverse of Ohm is Siemens
- Unit of resistivity is ohm-meter (Ω-m)
- Unit of conductivity is $(\Omega\text{-m})^{-1}$
- 27 orders of magnitude for electrical conductivity

- Metals ~ 10^7 $(\Omega\text{-m})^{-1}$
- Insulator ~ 10^{-10} - 10^{-20} $(\Omega\text{-m})^{-1}$
- Semiconductor ~ 10^{-6} - 10^4 $(\Omega\text{-m})^{-1}$
- Electrical conductivity depends on type of bonding, defect structure and temperature
- Flow of electrons from negative to positive potential
- Current flows in opposite direction
- Direct and Alternate current (DC and AC)

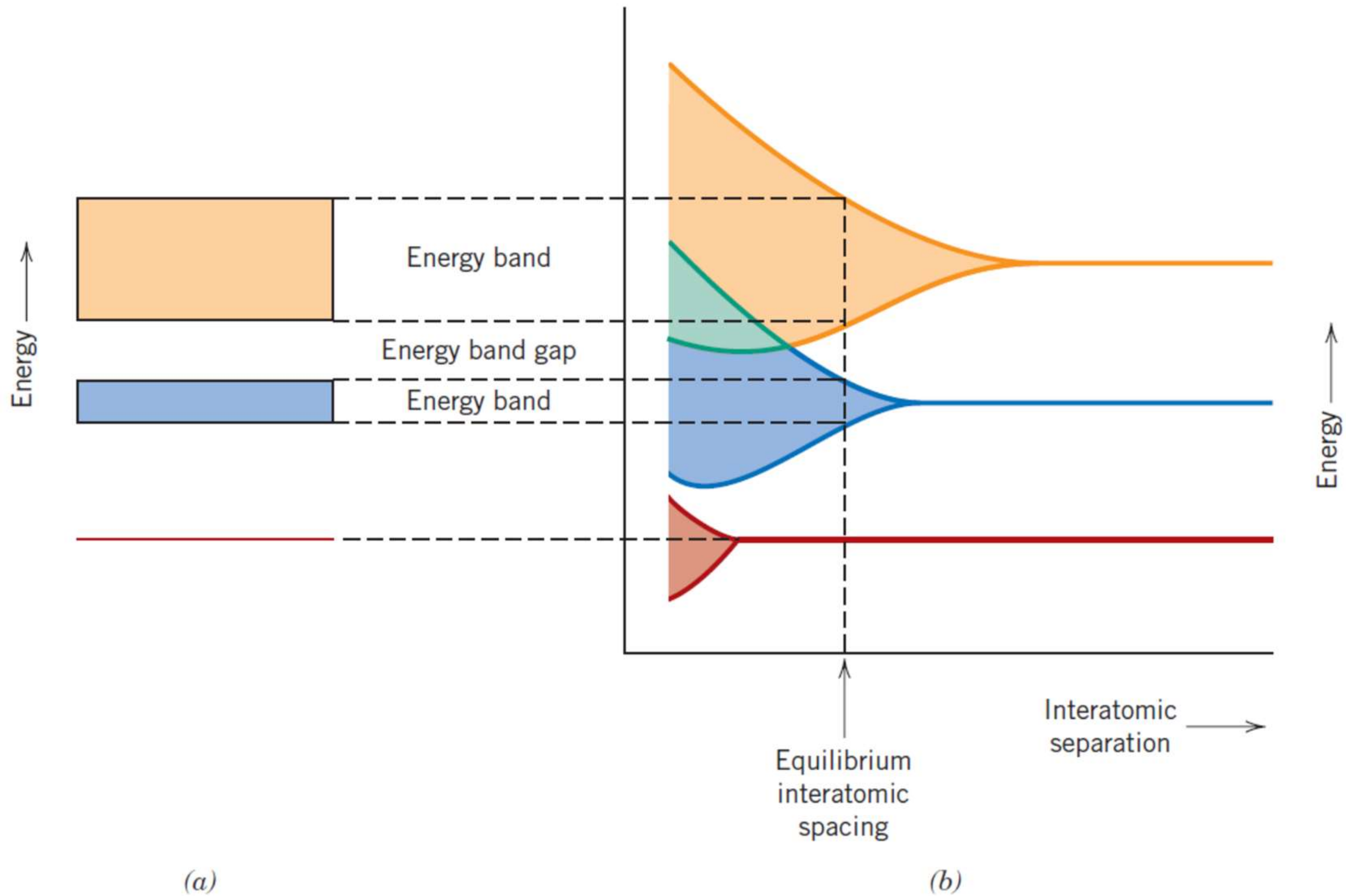
Band theory

- Electrons in atoms occupy different orbitals with different energy
- Energy states split into a series of energy states when more atoms are bought together to give rise to molecular orbitals
- These orbitals overlap to forms energy bands
- Long range and short range periodicity important
- Crystalline and amorphous materials
- Structure and energy bands are related

Splitting of energy levels

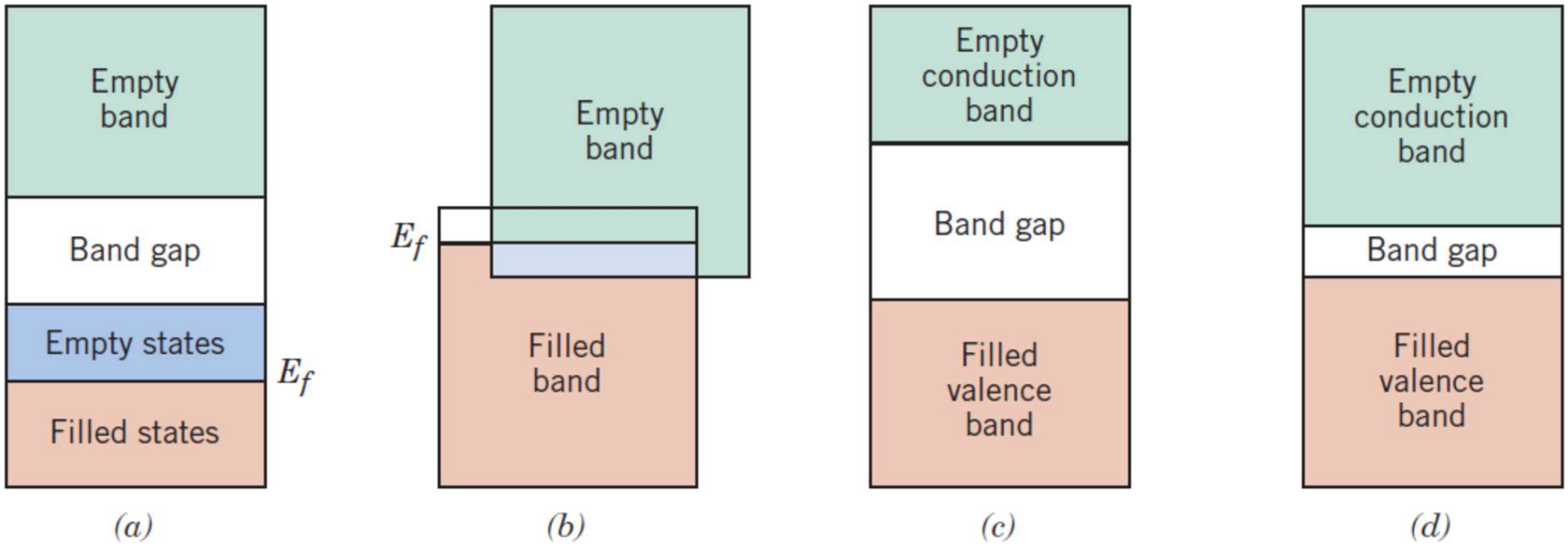


Formation of bands



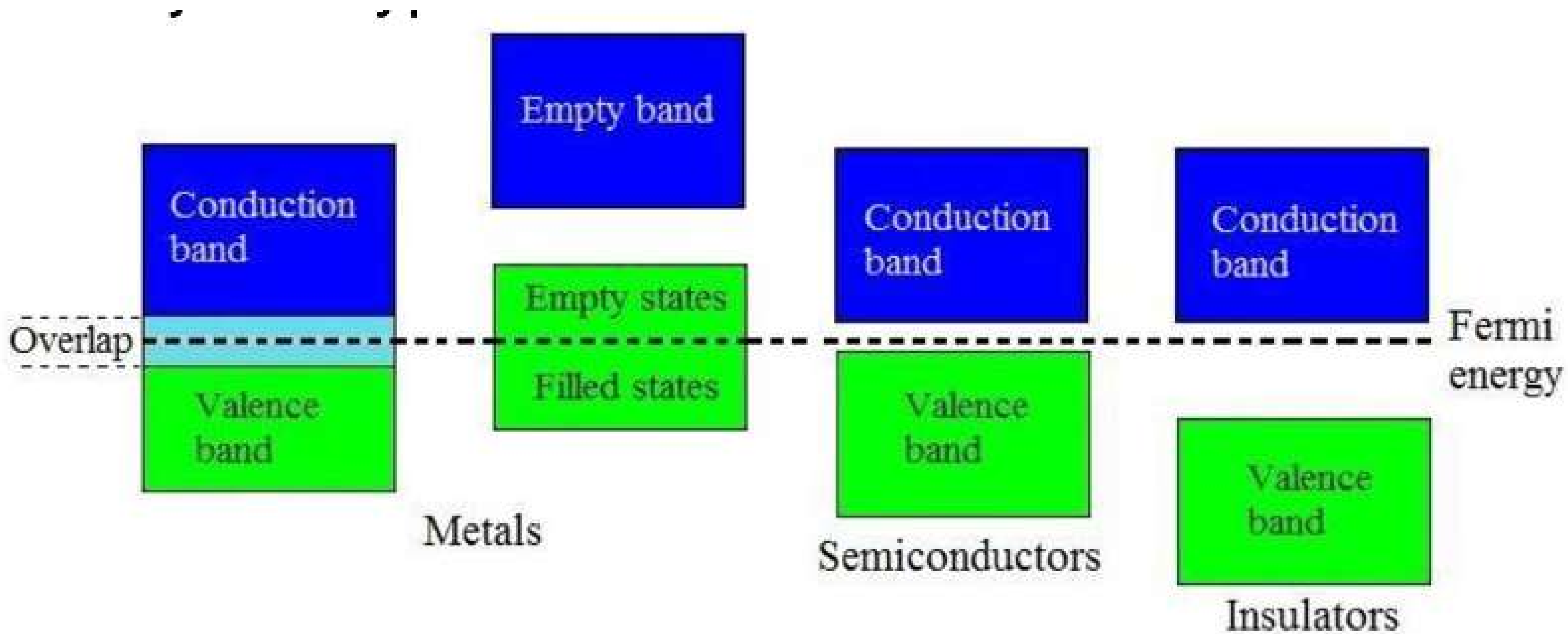
Band gap and class of materials

- The outermost or furthest band from the nucleus filled with valence electrons is called Valence band
- The empty band is called conduction band
- The energy of the highest filled state is called **Fermi energy**
- There is a gap between valence and conduction band
- Four distinct type of band structures in solids



- Metals have partially filled valence bands or overlapping valence and conduction band

- Semiconductors and insulators have completely filled valence band and empty conduction band to insulators



- The magnitude of band gap decides electronic character
- Smaller bandgap in semiconductor compared to insulators

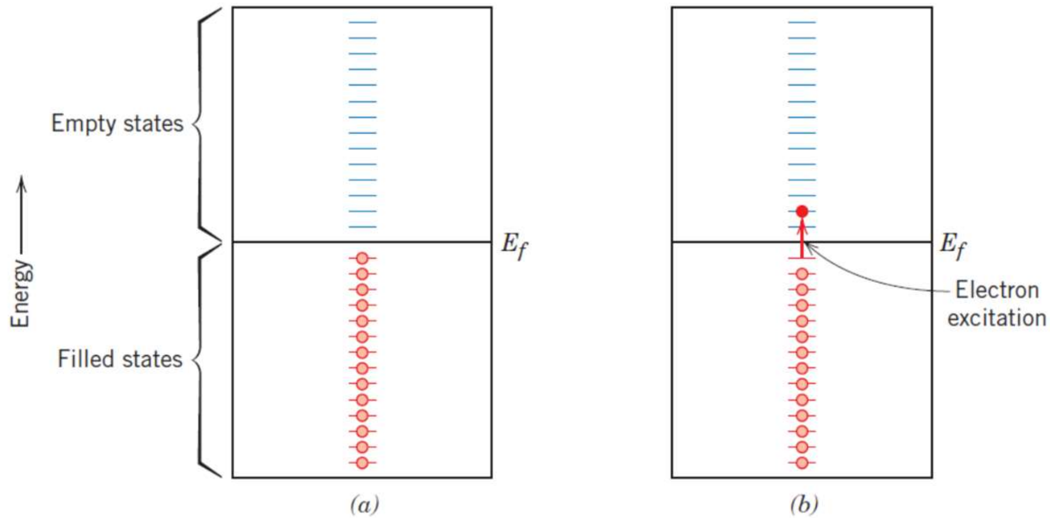
Conduction mechanism

- Electron has to be excited from the filled state to the empty state above the Fermi level to become a free electron from a bound electron

- Free electron is a charge carrier

- Metals have large free electrons in the valence state and they can be easily excited to the empty states above Fermi level

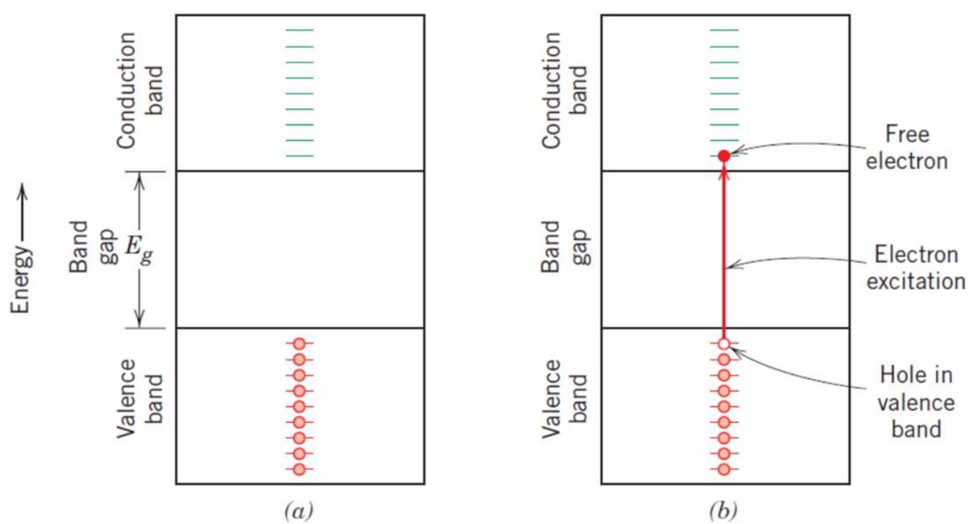
- Large energy is required to do the same in semiconductors and particularly in insulators



Metallic bonding

Electron gas

Electrons free to move from VB to CB



Covalent or ionic bonding

Electron hole pair generation in semiconductors

Weak covalent for semiconductors small bandgap compared to insulators

Electron mobility and conductivity

Drift velocity is the average electron velocity in the direction of the force exerted by the electric field

$$v_d = \mu_e \mathscr{E}$$

Scattering of electrons at different length scales

Electron mobility μ_e is an indication of scattering events for electrons

$$\sigma = n|e|\mu_e$$

Factors influencing resistivity

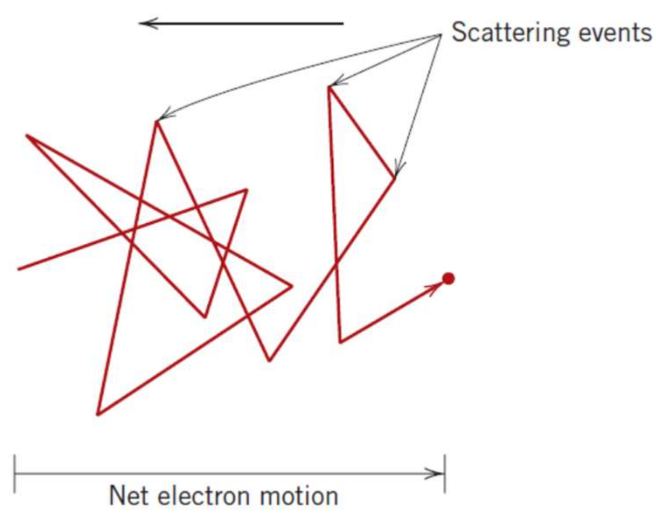
Temperature, impurity and defects $\rho_{\text{total}} = \rho_t + \rho_i + \rho_d$

More defects like dislocations and grain boundaries in crystalline materials more scattering less conductivity

Thermal scattering with increase in temperature $\rho_t = \rho_0 + aT$

$$\rho_i = Ac_i(1 - c_i)$$

$$\rho_i = \rho_\alpha V_\alpha + \rho_\beta V_\beta$$



Ionic conductivity

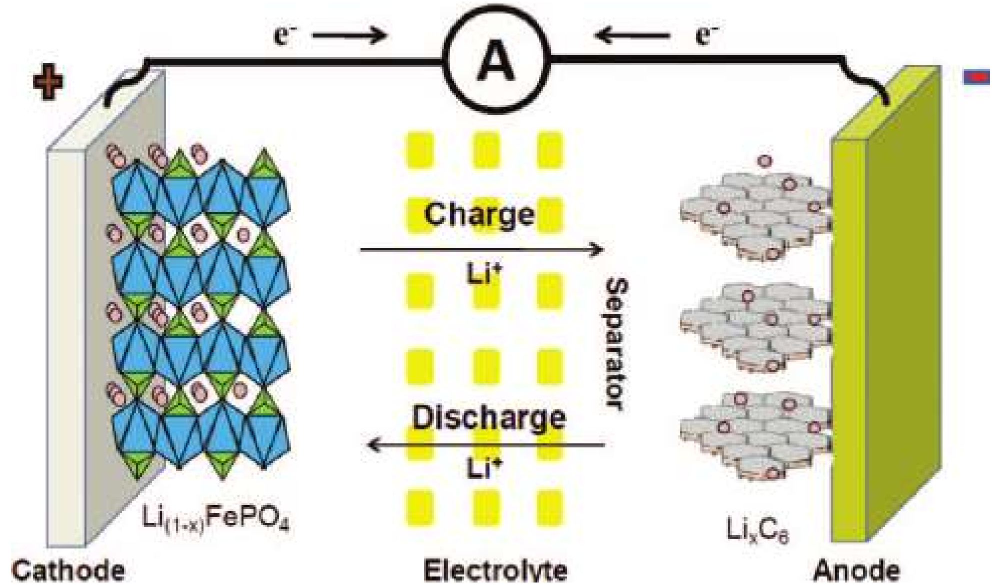
- Ions instead of electrons
- Mass transfer along with charge transfer
- Conductivity decreases as temperature decreases exponentially
- Schottky and Frenkel defects
- Batteries, fuel cells, gas sensors
- AgI, Na^+ doped beta alumina, $LiCoO_2$, ZrO_2, PbF_2

$$\sigma_{\text{total}} = \sigma_{\text{electronic}} + \sigma_{\text{ionic}}$$

$$\mu_I = \frac{n_I e D_I}{kT}$$

https://www.slideserve.com/seth/ionic-conductivity-and-solid-electrolytes-i-the-basics

The ubiquitous Li ion battery



Can we make batteries that require no charging ?
Impossible, well work is going for development of nuclear batteries.
Driverless cars and reusable rockets are already here so who knows, it may happen in our life time

https://www.tandfonline.com/doi/full/10.1080/15583724.2011.593390

Intrinsic semiconductors

- Column IV elements like Si and Ge are intrinsic elemental semiconductors
- Column III and V compounds like GaN, GaAs, GaP
- Column II and VI compounds like ZnS, InSb, CdTe
- Ternary GaAsP and quaternary InGaAsP

Intrinsic semiconductors

- Bandgap upto 2 eV for semiconductors
- Easy to excite electron from valence to conduction band
- Excited electron leaves behind a hole in the valence band
- An electron can move to a hole under an electrical potential so hole is also a charge carrier
- Mobility of electrons and holes decide electronic properties of semiconductors

Table 18.3 Band Gap Energies, Electron and Hole Mobilities, and Intrinsic Electrical Conductivities at Room Temperature for Semiconducting Materials

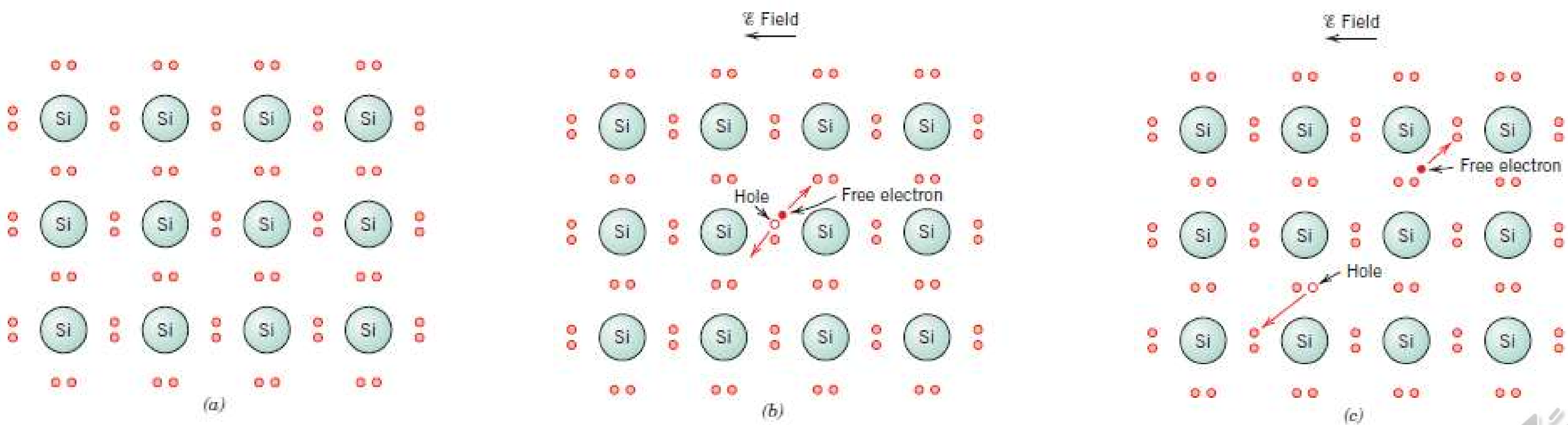
Material	*Band Gap* (eV)	*Electrical Conductivity* $[(\Omega \cdot m)^{-1}]$	*Electron Mobility* ($m^2/V \cdot s$)	*Hole Mobility* ($m^2/V \cdot s$)
		Elemental		
Si	1.11	4×10^{-4}	0.14	0.05
Ge	0.67	2.2	0.38	0.18
		III–V Compounds		
GaP	2.25	—	0.03	0.015
GaAs	1.42	10^{-6}	0.85	0.04
InSb	0.17	2×10^{4}	7.7	0.07
		II–VI Compounds		
CdS	2.40	—	0.03	—
ZnTe	2.26	—	0.03	0.01

Conductivity and carrier mobility

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

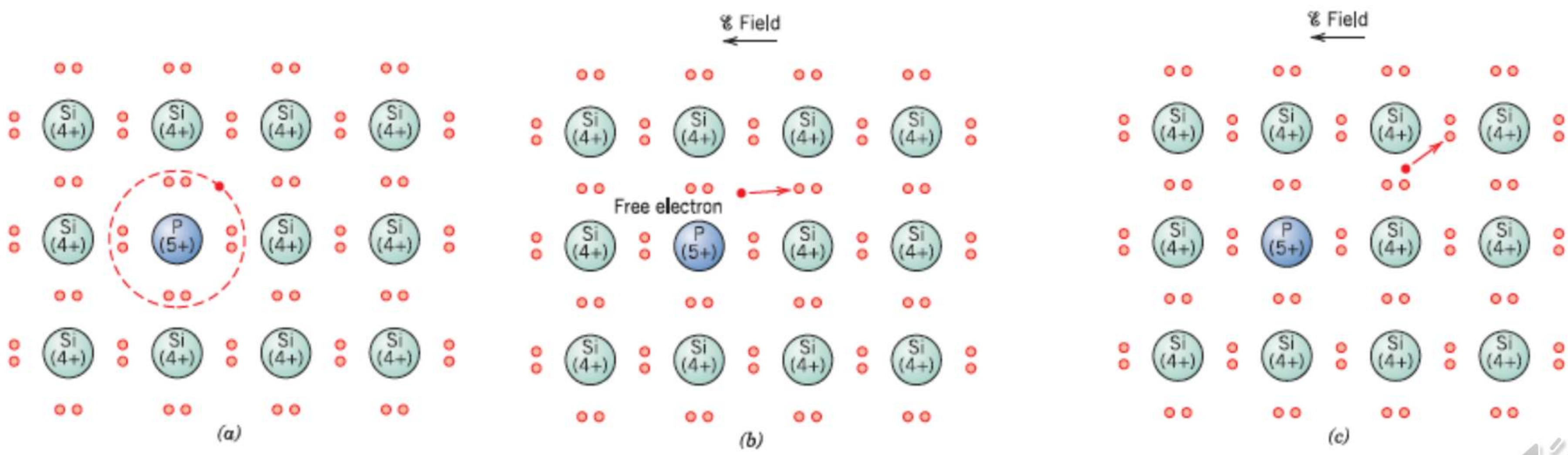
$$n = p = n_i$$

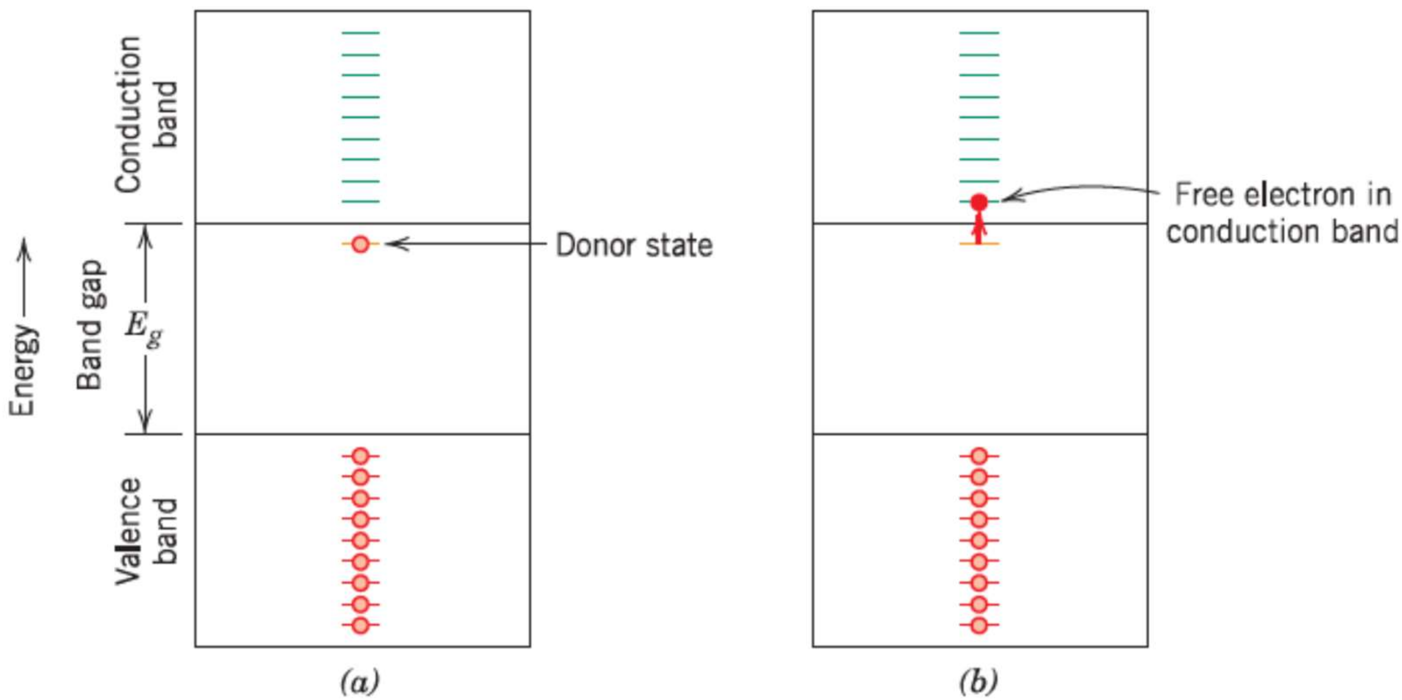
$$\sigma = n|e|(\mu_e + \mu_h) = p|e|(\mu_e + \mu_h) = n_i|e|(\mu_e + \mu_h)$$



Extrinsic n-type semiconductors

- Doping of Group VA like P, As, Sb, Bi in Si/Ge
- Extra electron with low binding energy
- Creation of donor state in bandgap close to CB
- Can be easily taken to CB n >> p





$$\sigma \cong n|e|\mu_e$$

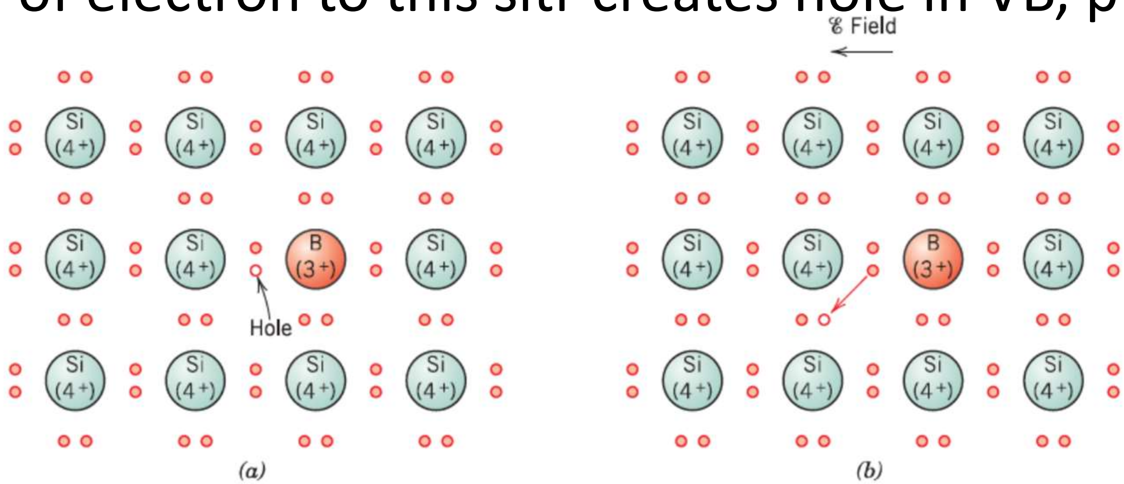
Extrinsic p-type semiconductors

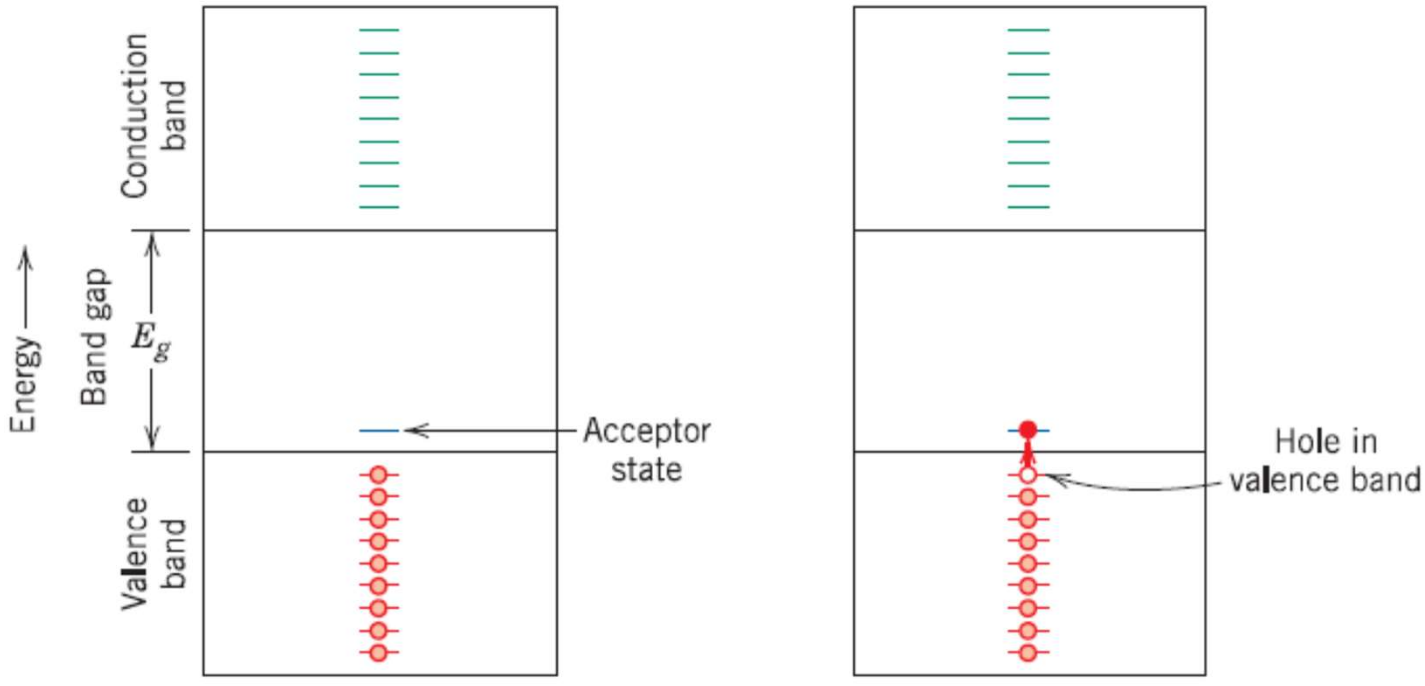
- Doping of Group IIIA like Al, B, Ga to Si/Ge

- One less electron, missing electron or hole

- Each dopant atom introduces an energy level in the band gap very close to VB

- Transfer of electron to this sitr creates hole in VB, p >> n



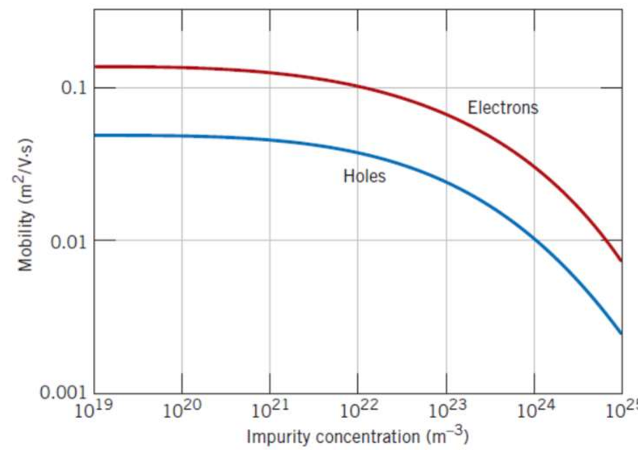


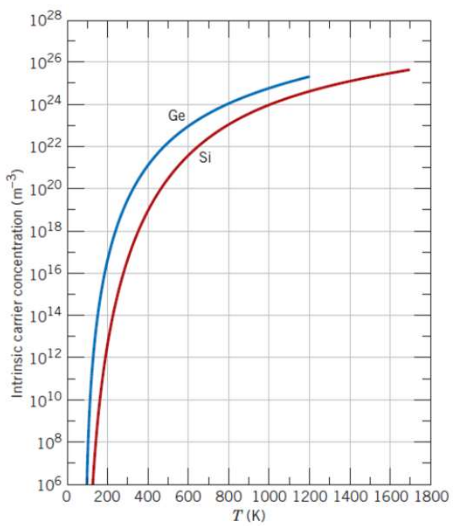
(a) (b)

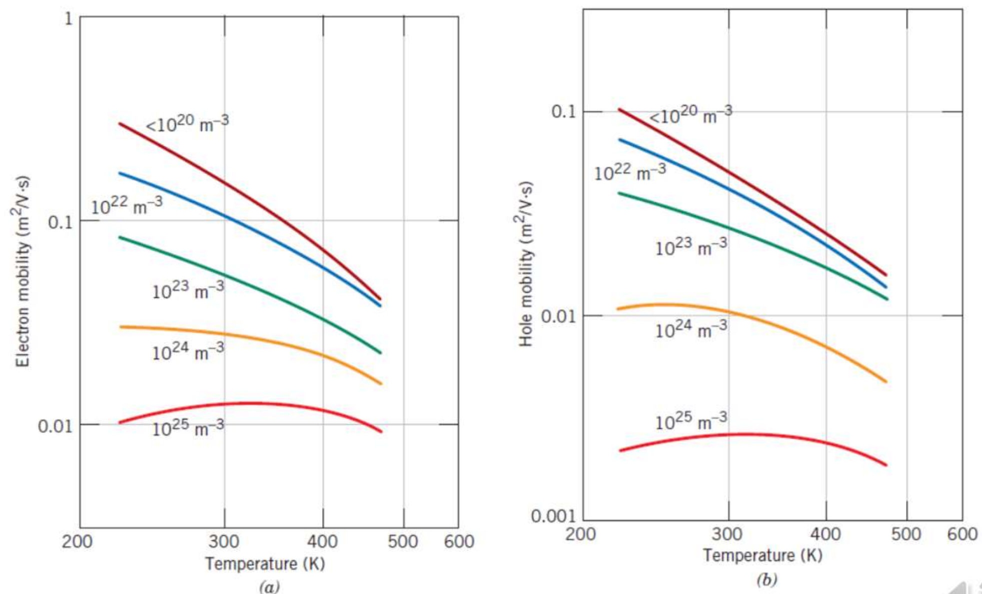
$$\sigma \cong p|e|\mu_h$$

Factors influencing carrier mobility

- Dopant concentration
- Temperature
- Carrier concentration increases with temperature







Semiconductor physics

- Wave particle duality of electrons
- Describe wave functions in valence and conduction bands
- Concept of effective mass of electron as the free electron interacts with periodic lattice potential in CB
- Band gap can be overcome by absorbing a photon
- Similar analogy for holes or missing electrons
- Thermal generation and recombination of electron and holes in absence of radiation

Quantum mechanics

- Density of states is the number of electronic states or electron wavefunctions in a band per unit energy per unit volume of a crystal

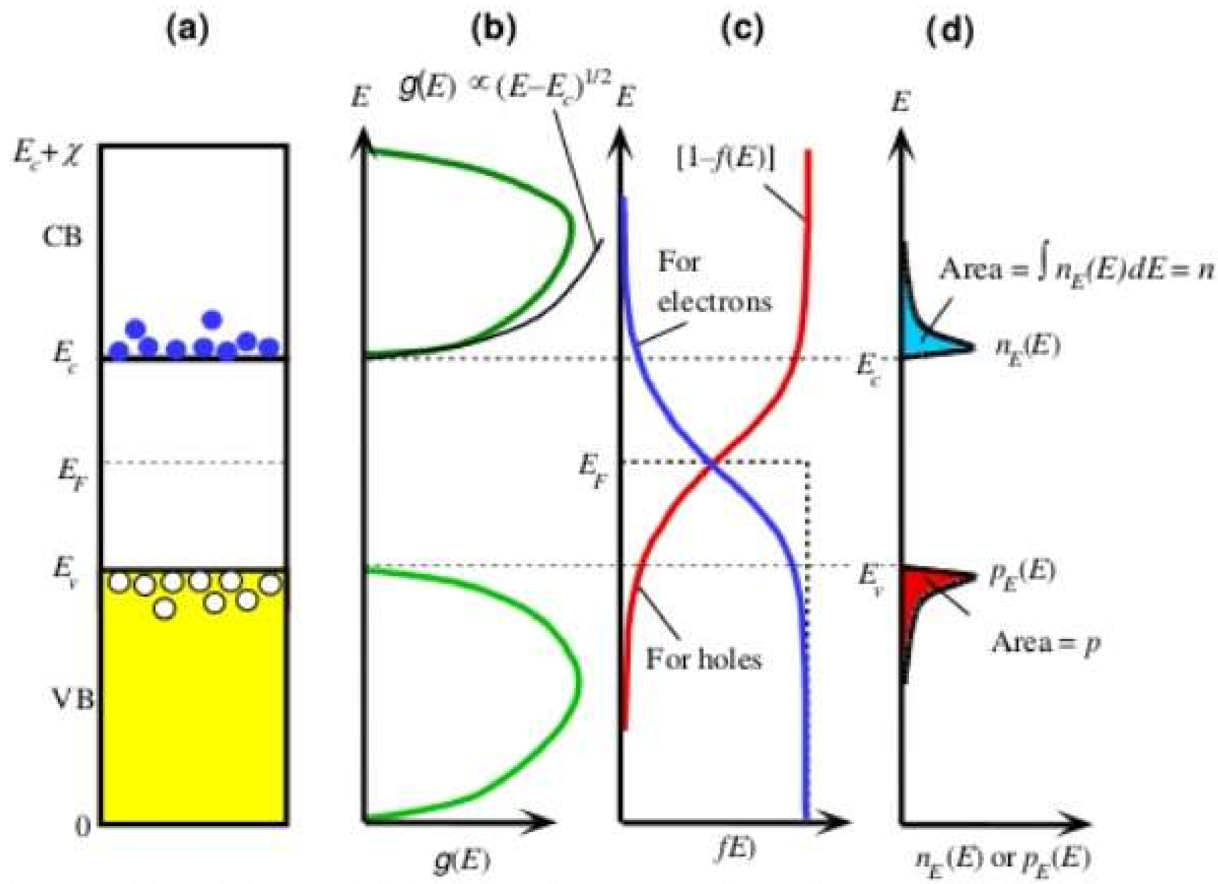
- Quantum mechanics and fermi energy as related to electron concentration in CB and hole concentration in VB

- Electron trapped in a potential well

- Periodic potential of crystal

- Energy versus crystal momentum or E-k plots

Energy-momentum or E-k diagram



(a) Energy band diagram. (b) Density of states (number of states per unit energy per unit volume). (c) Fermi-Dirac probability function (probability of occupancy of a state). (d) The product of $g(E)$ and $f(E)$ is the energy density of electrons in the CB (number of electrons per unit energy per unit volume). The area under $n_E(E)$ vs. E is the electron concentration.

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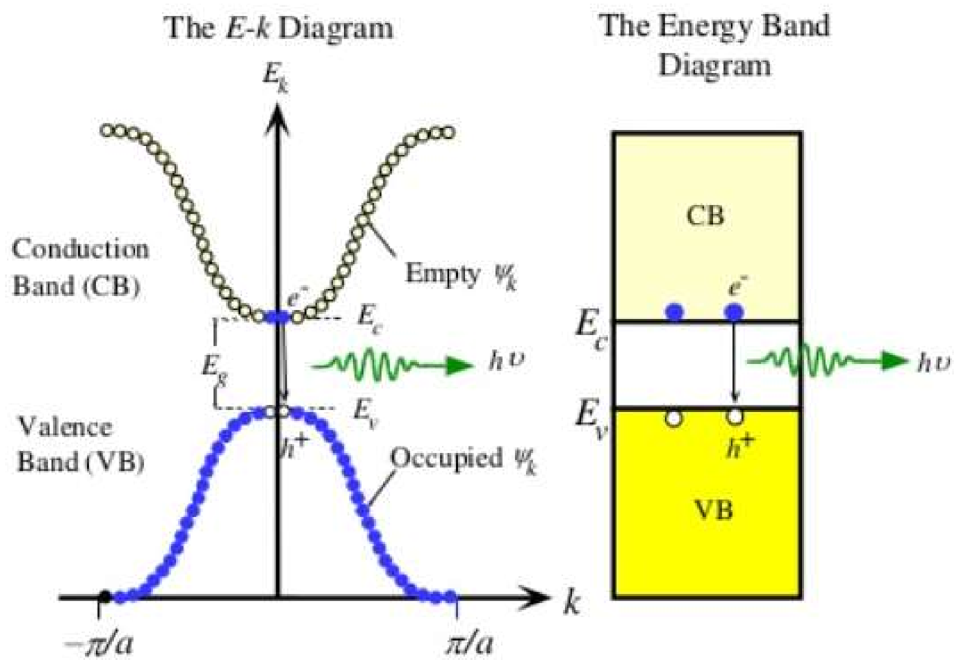

The E-k diagram of a direct bandgap semiconductor such as GaAs. The E-k curve consists of many discrete points with each point corresponding to a possible state, wavefunction $\psi_k(x)$, that is allowed to exist in the crystal. The points are so close that we normally draw the E-k relationship as a continuous curve. In the energy range E_v to E_c there are no points ($\psi_k(x)$ solutions).

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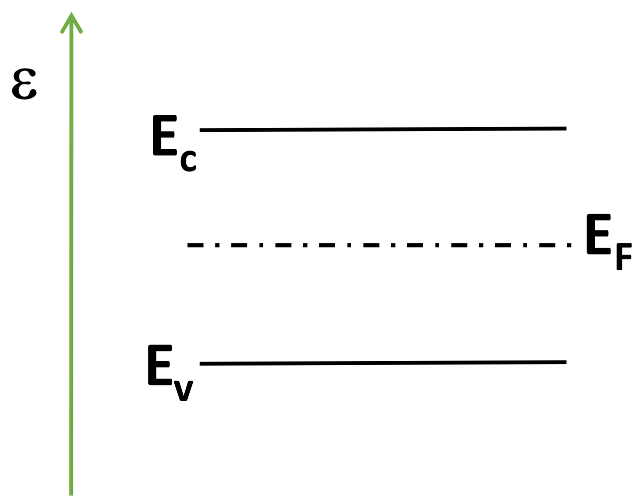
For intrinsic semiconductors, at thermal equilibrium with bandgap E_g

$$n = p = \mathrm{n_i} = (N_c N_v)^{1/2} \exp\left[-\left(\frac{E_g}{2k_B T}\right)\right]$$

For extrinsic n-type semiconductors, at thermal equilibrium



$$\mathrm{n} = \mathrm{n_i} = N_c \exp\left[-\left(\frac{E_g}{k_B T}\right)\right]$$

Direct and Indirect bandgap semiconductors

- Only change in energy is required for electron to move from VB to CB for direct bandgap while change in momentum and energy for indirect bandgap semiconductor

- GaAs is direct bandgap while Si and Ge are indirect bandgap

- Probability of radiation induced transition higher in direct bandgap semiconductors

- Higher efficiency and mostly used for optical devices