Semiconductor Devices (EE336)

Lec. 2: Energy Bands and Charge Carriers

Wed. Oct. 5th, 2016

Dr. Mohamed Hamdy Osman

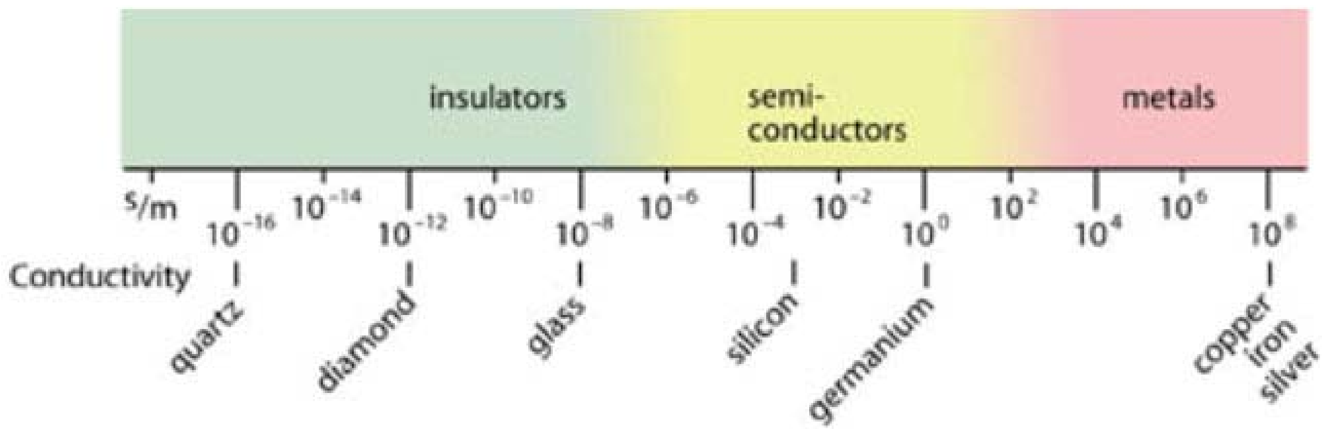
Lecture Outline

- What is a semiconductor? & Semiconductor materials
- Electronic configuration of Si atom
- Si crystal and covalent bonding
- Formation of energy bands and gaps in solid crystals
- Energy band diagram and measurement of energy gap
- Metals, insulators and semiconductors

What is a semiconductor?

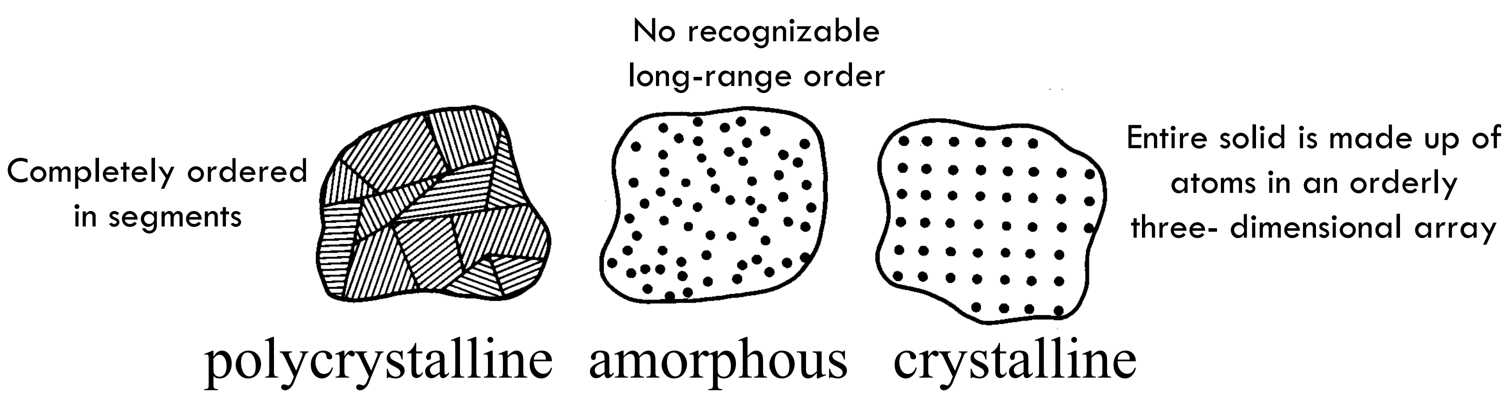
- Low resistivity ⇒ "conductor"
- High resistivity ⇒ "insulator"
- Intermediate resistivity ⇒ "semiconductor"

- The conductivity (S/m) and at the same time the resistivity of semiconductors lies between that of conductors and insulators.



What is a semiconductor?

- Semiconductors are some of the purest solid materials in existence, because any trace of impurity atoms called "*dopants*" can change the electrical properties of semiconductors drastically.
- Unintentional impurity level:
  1 impurity atom per 10^9 semiconductor atom or 1 part per billion (ppb) (Electronic grade Si)
- Intentional impurity ranging from 1 per 10^8 to 1 per 10^3 (via doping)



- Most devices fabricated today employ crystalline semiconductors.

Semiconductor materials

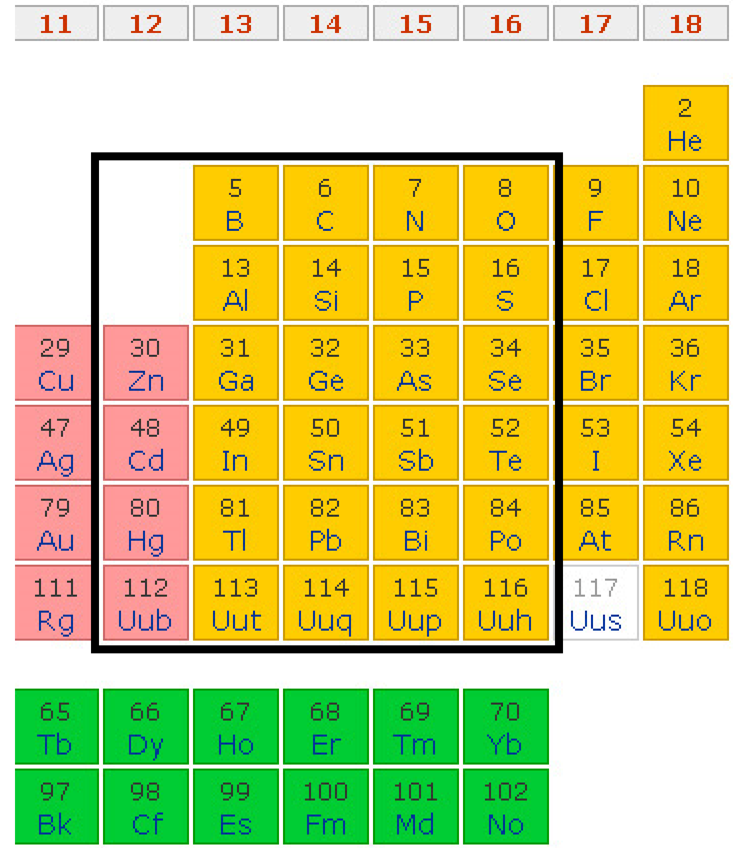
Elemental: Si, Ge, C (tetravalent)

Compound: III-V GaAs, GaN (trivalent + pentavalent)

II-VI CdSe

Alloy: $Si_{1-x}Ge_x$

$Al_xGa_{1-x}As$



As : Arsenic
Cd : Cadmium
Se : Selenium
Ga : Gallium

Recall four quantum numbers

Quantum Numbers

$n = 1, 2, 3, \ldots$

$l = 0, 1, 2, \ldots, n-1$

$m = -l, \ldots, -1, 0, 1, \ldots, l$

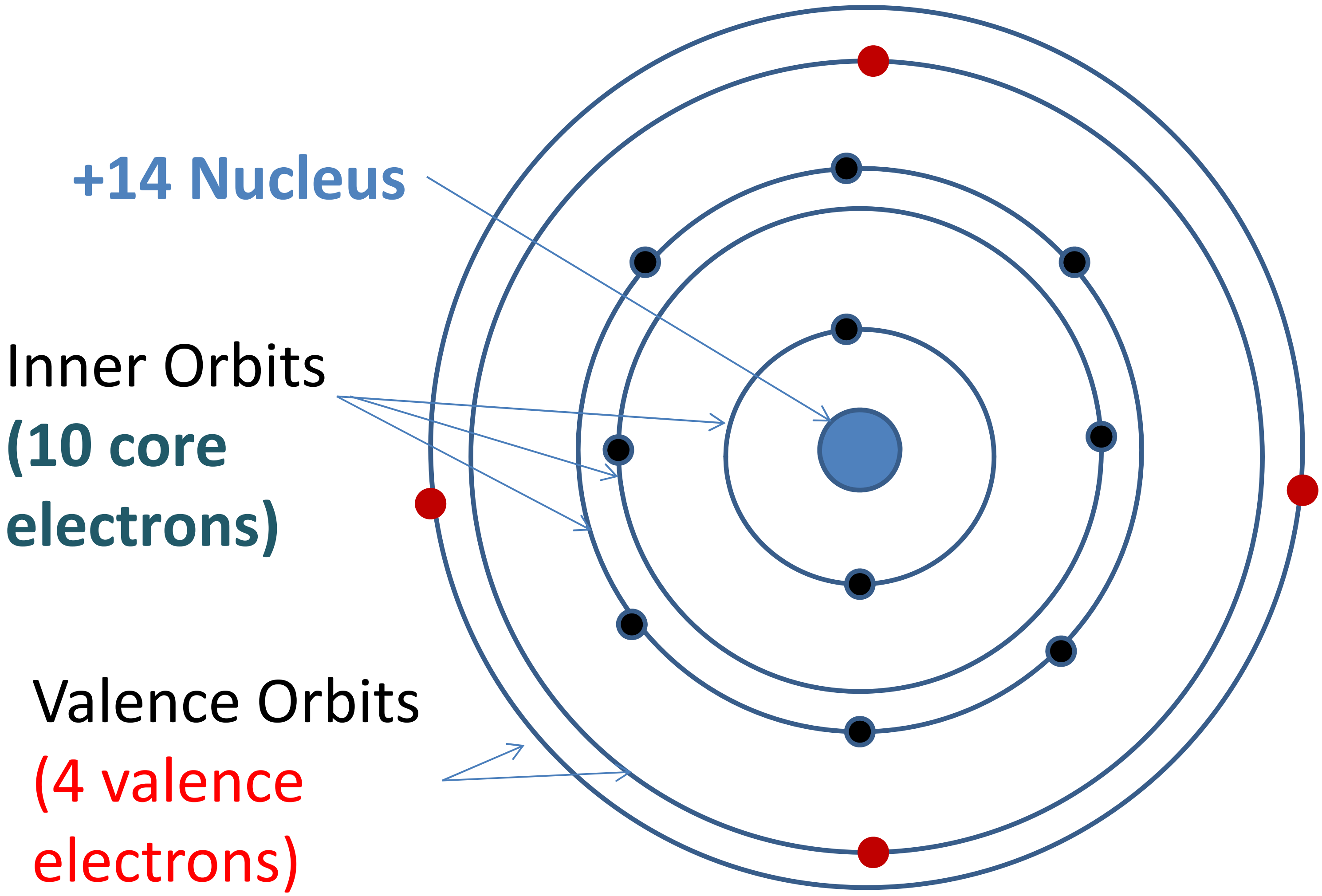
$s = \pm\frac{1}{2}$

- Standard notation for electronic configuration

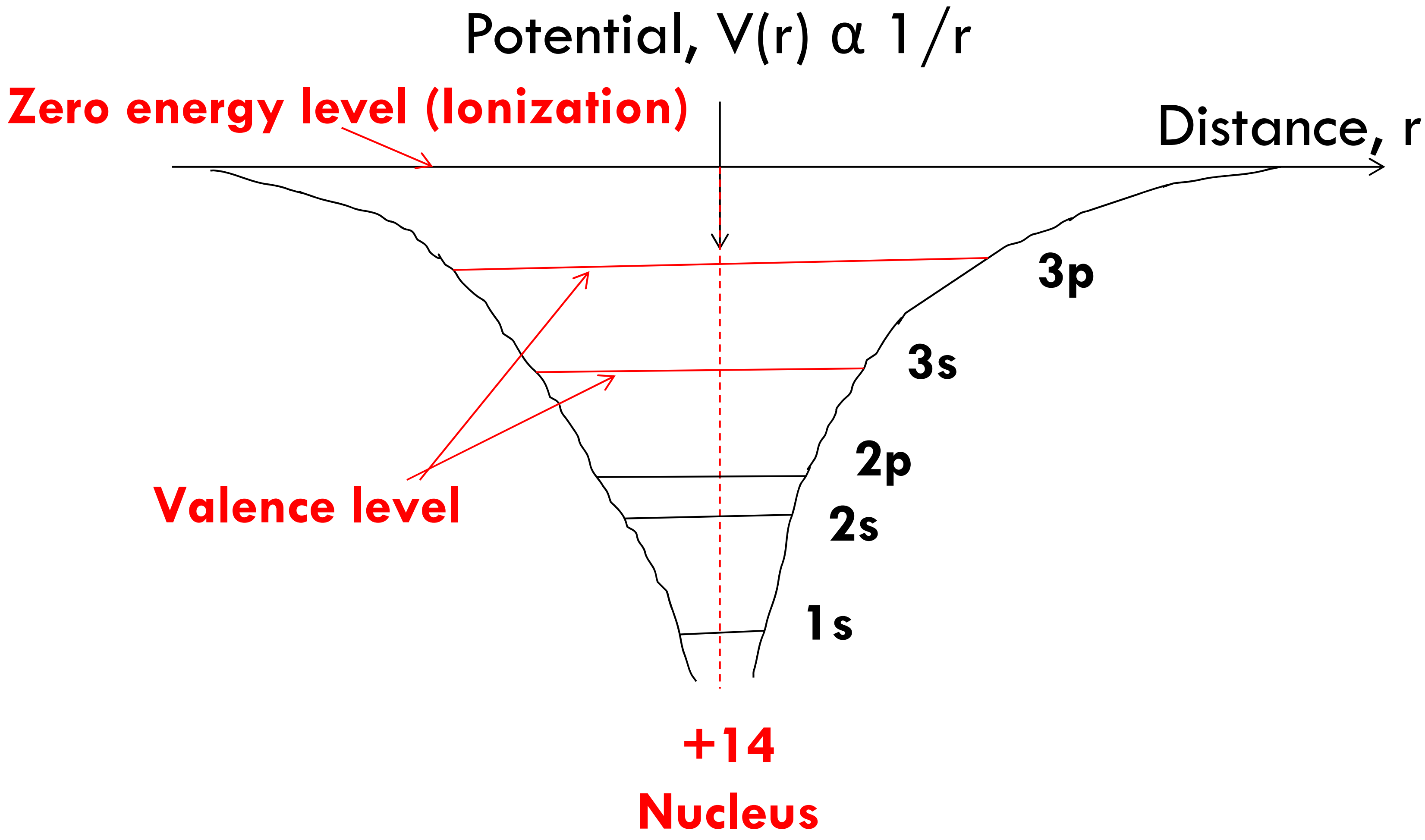
$l = 0 \rightarrow s$ $l = 1 \rightarrow p$ $l = 2 \rightarrow d$ $l = 3 \rightarrow f$

Electronic configuration of Si

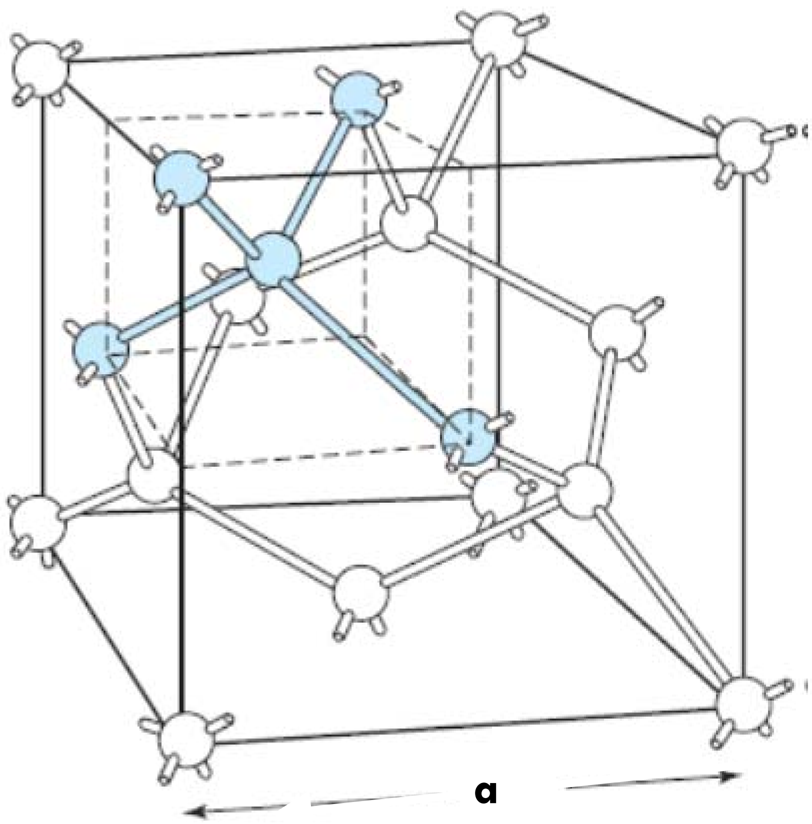
For Si with Z = 14 → $1s^2 2s^2 2p^6 3s^2 3p^2$ → [Ne] $3s^2 3p^2$



Energy levels of Si atom in Columbic potential well



Si Crystal



"Diamond Lattice"

- **Each Si atom has 4 nearest neighbors.**
- **Atom lattice constant**
  (length of the unit cell side)
  $a = 5.431 \text{Å}$, $1 \text{Å} = 10^{-10}$ m

- **Each cell contains:**
  - **8 corner atoms**
  - **6 face atoms**
  - **4 interior atoms**

Si Crystal

- **Number of atoms in a unit cell:**
  - 4 atoms completely inside cell
  - Each of the 8 atoms on corners are shared among 8 cells → count as 1 atom inside cell
  - Each of the 6 atoms on the faces are shared among 2 cells → count as 3 atoms inside cell
  - ⇨ Total number inside the cell = 4 + 1 + 3 = **8**

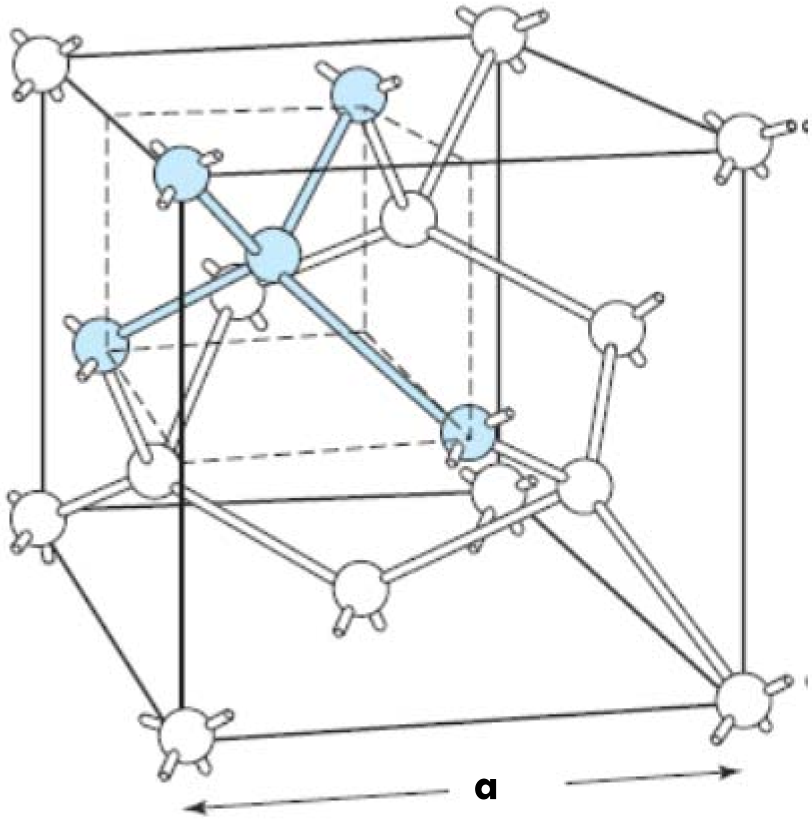
- **Cell volume** = $(.543\ \text{nm})^3 = 1.6 \times 10^{-22}\ \text{cm}^3$
- **Density of silicon atom**

  = (8 atoms) / (cell volume)

  = $\mathbf{5 \times 10^{22}}$ **atoms/cm^3**

- **What is density of silicon in g/cm^3? (see Example 1.3 in Streetman)**

Si Crystal



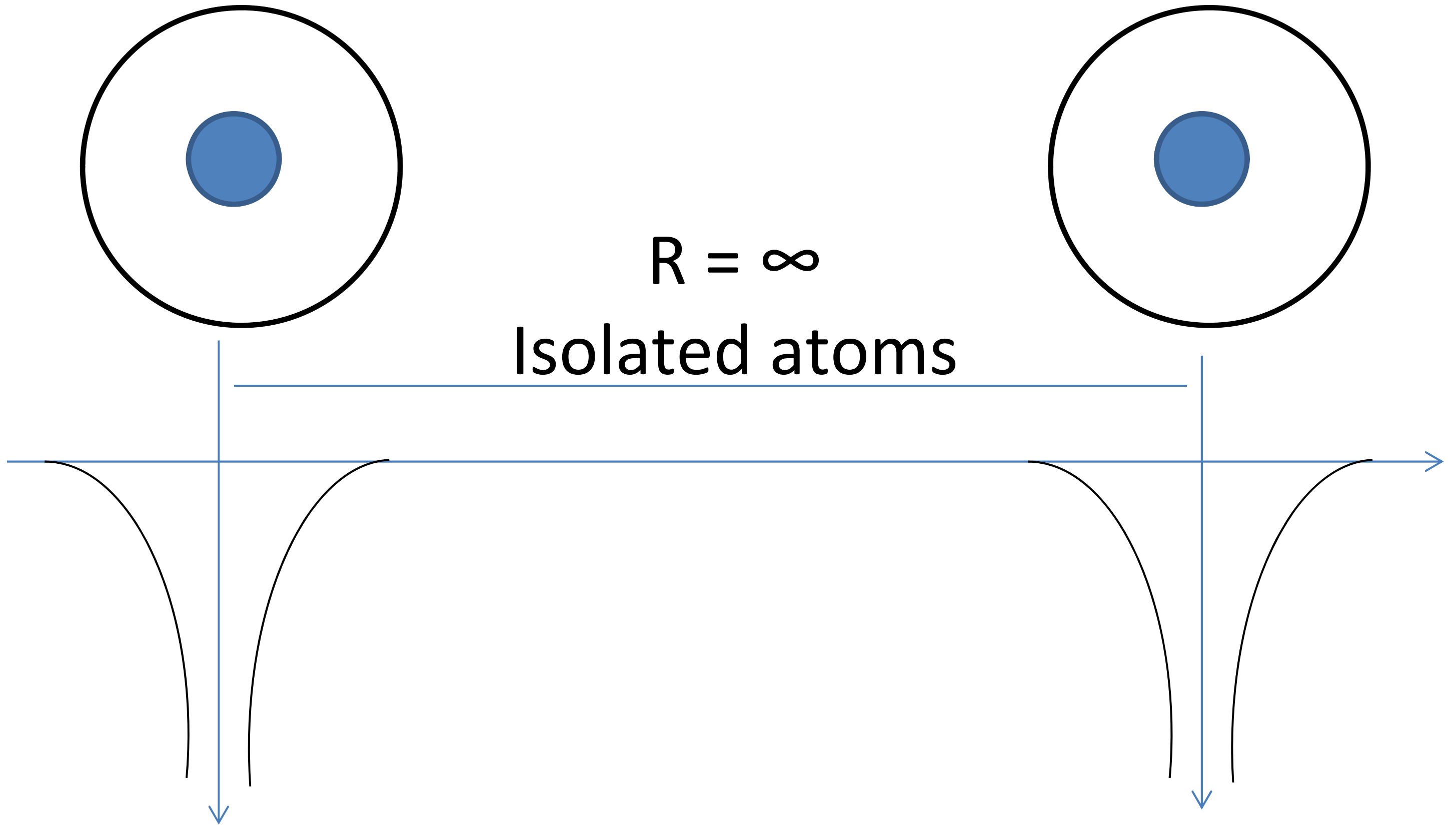
"Covalent bond between every two nearest neighbors within Si crystal"

- ***Two electrons participate in every bond***
- ***Once bonding is established, it is no longer relevant to ask which electron belongs to which atom***

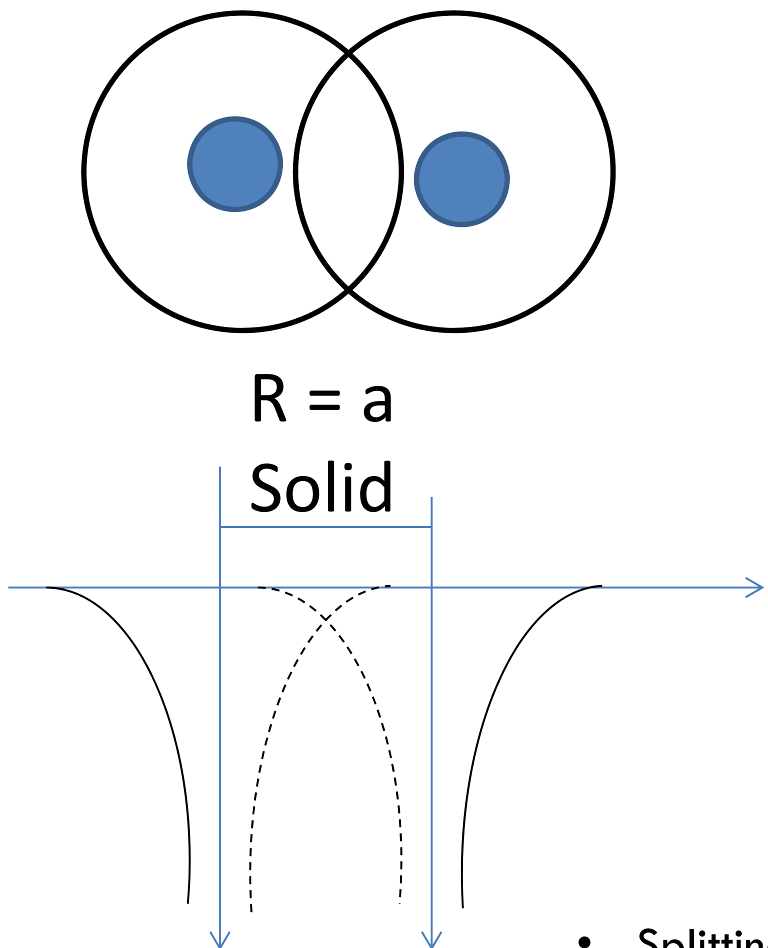
Why chemical bonding occurs and what happens?

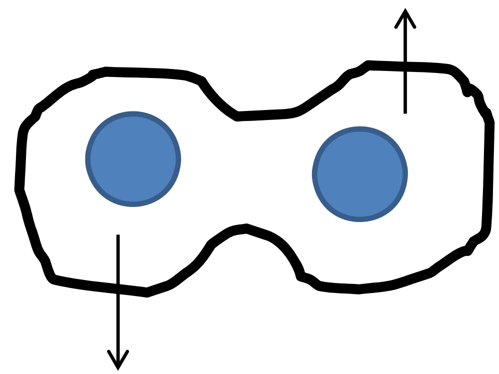
- A ***chemical bond*** is an increase in electron density along or to the sides of the connecting line between the nuclei
- There are different types of bonding such as ionic bonding, covalent bonding, etc.
- In order for a chemical bond to be stable, there must be energy favoring compared to the case where bonding does not occur, i.e. electrons constituting the bond will fill lower energy levels relative to the isolated case
- In order to qualitatively understand why bonding occurs, we will use the concept of **hybridization** via **linear combination of atomic orbitals (LCAO)**

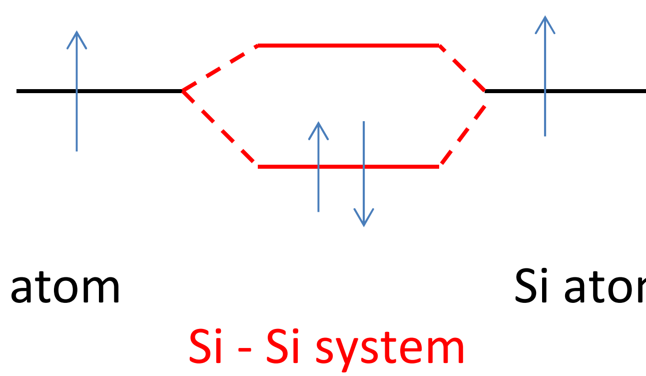
Why chemical bonding occurs and what happens?



Why chemical bonding occurs and what happens?

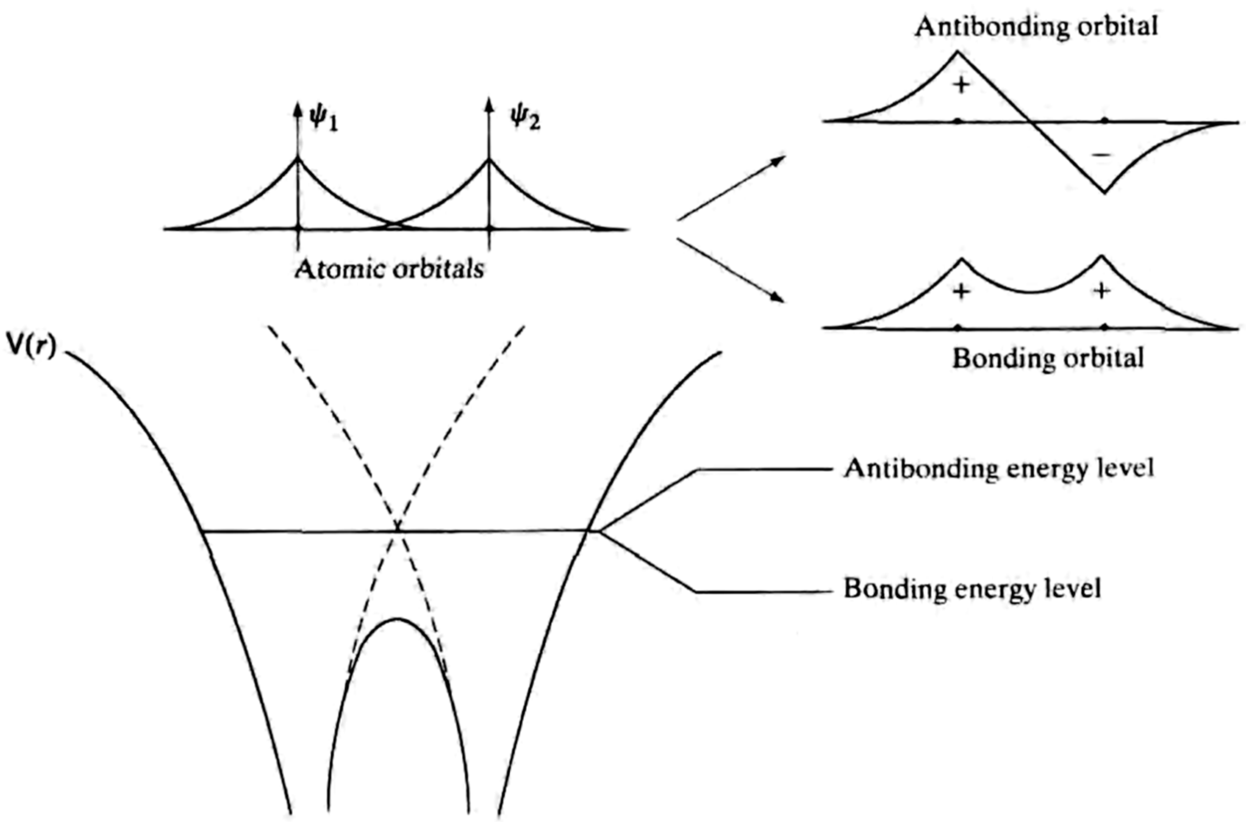






- Splitting of two identical orbitals into two bonding and antibonding orbitals
- Two electrons will fill the lower energy bonding state with opposite spin

Why chemical bonding occurs and what happens?

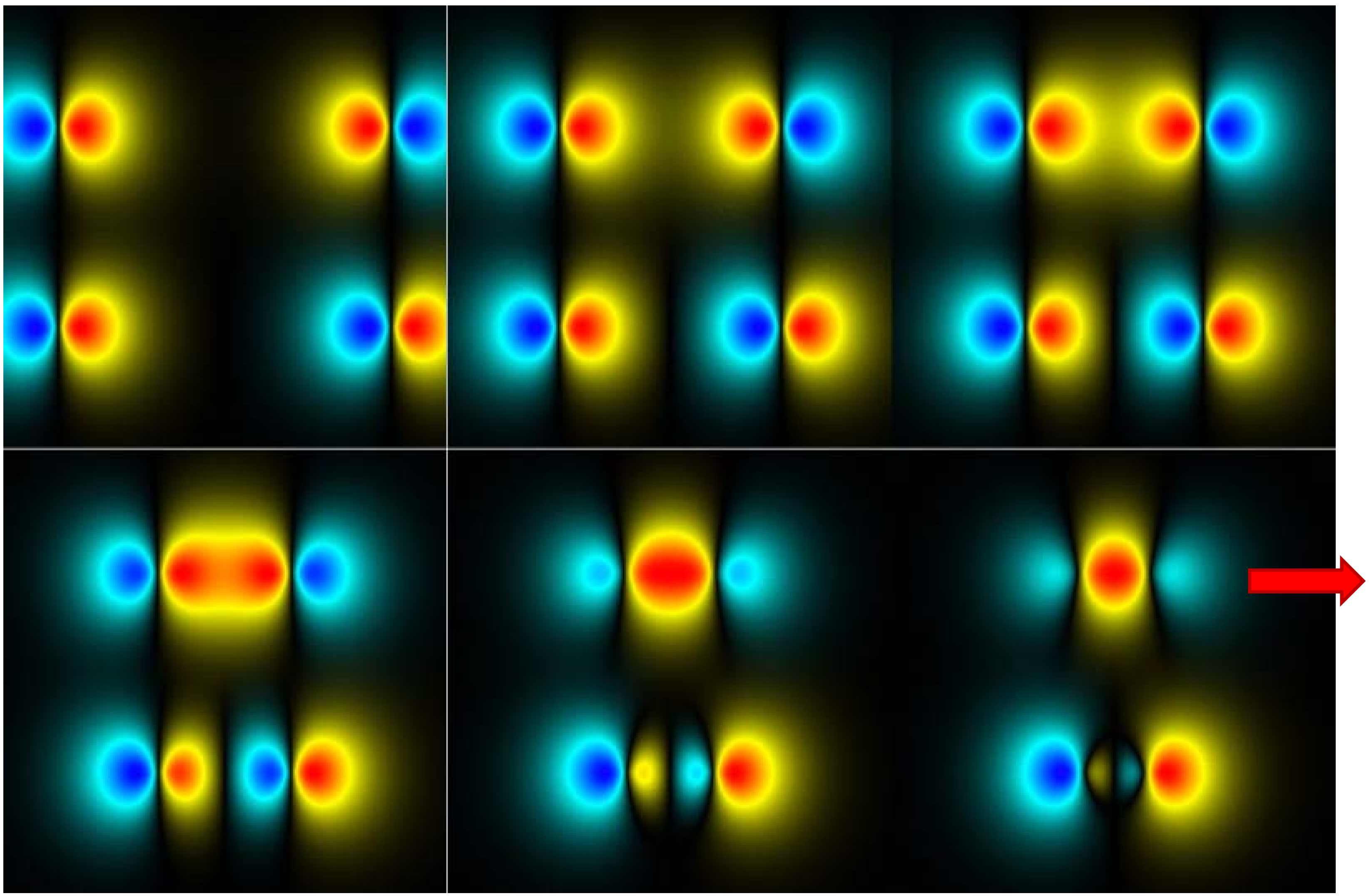


$$\psi_1 - \psi_2$$

$$\psi_1 + \psi_2$$

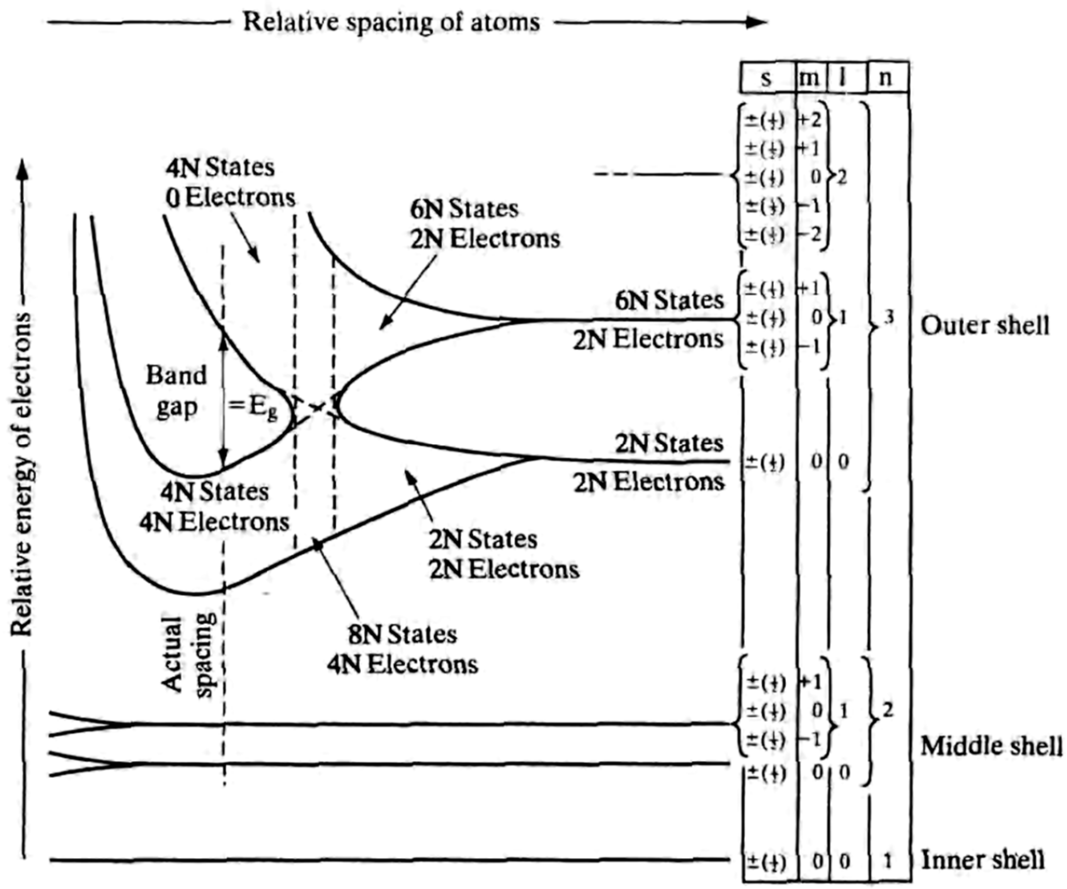
Has higher probability in the zone between the two atoms

Why chemical bonding occurs and what happens?



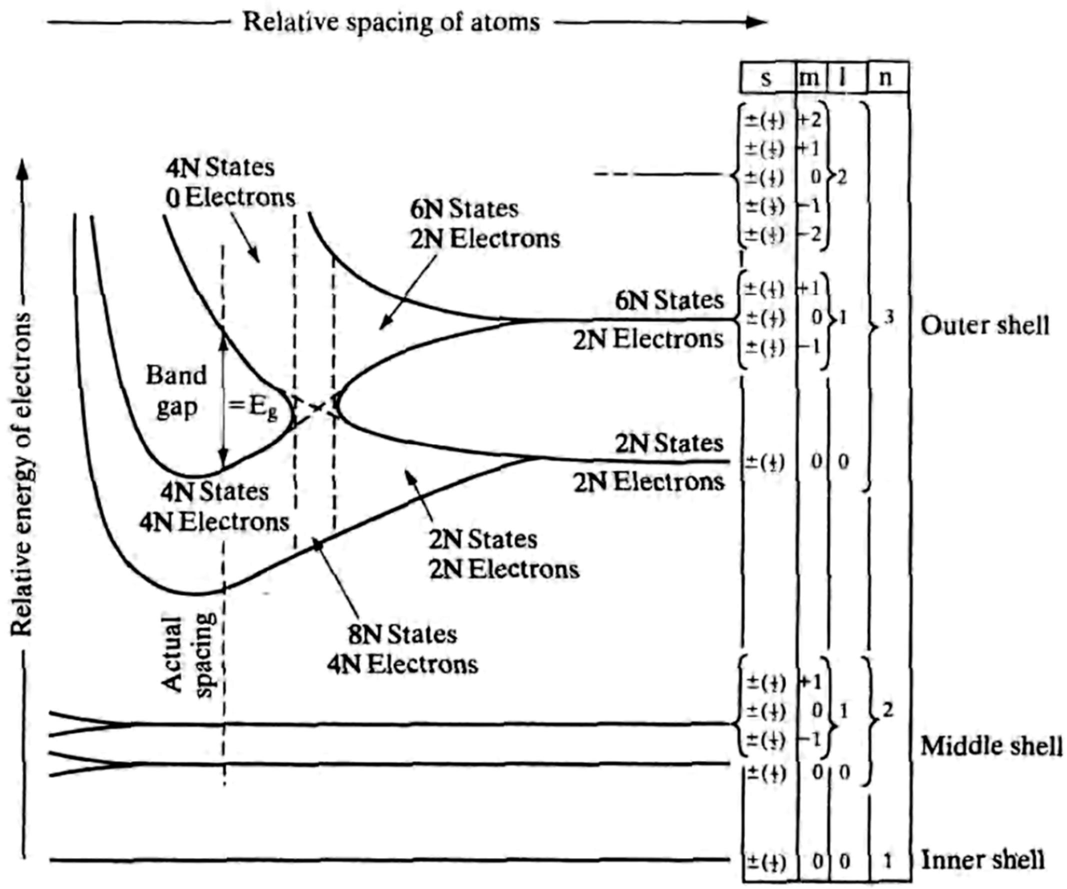
Has higher probability in the zone between the two atoms

Formation of energy bands and energy gap in Si crystal



- For isolated atoms, 2N states of type 3s filled with 2N electrons and 6N states of type 3p filled with 2N electrons
- As atomic spacing decreases, energy levels split and form bands
- At the actual atomic spacing, there are two bands (called valence and conductions bands) separated by an energy gap E_g

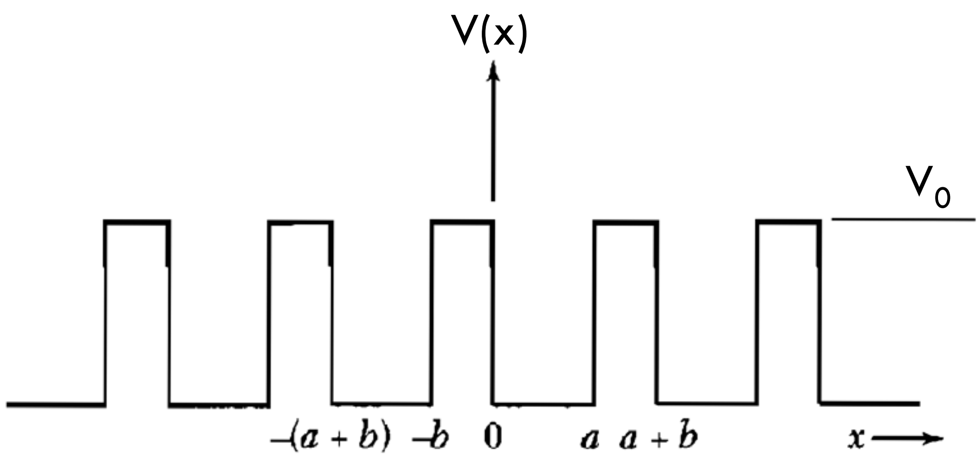
Formation of energy bands and energy gap in Si crystal

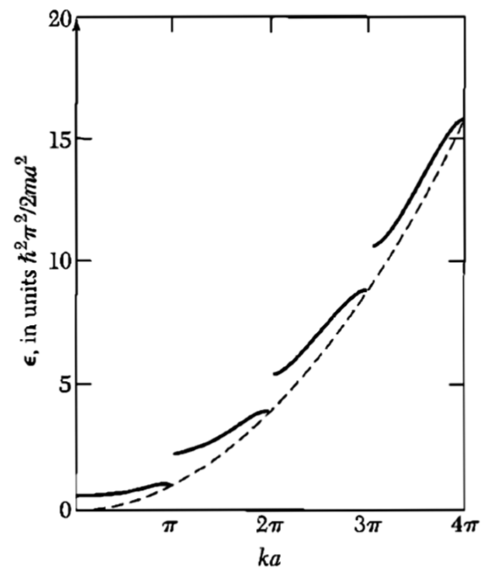


- The valence band has 4N states filled with 4N electrons (at 0 K) because electrons tend to fill the lowest possible energy states
- The conduction band has 4N states that are totally empty at 0 K, i.e. under no thermal excitation

Formation of energy bands and energy gap in Si crystal

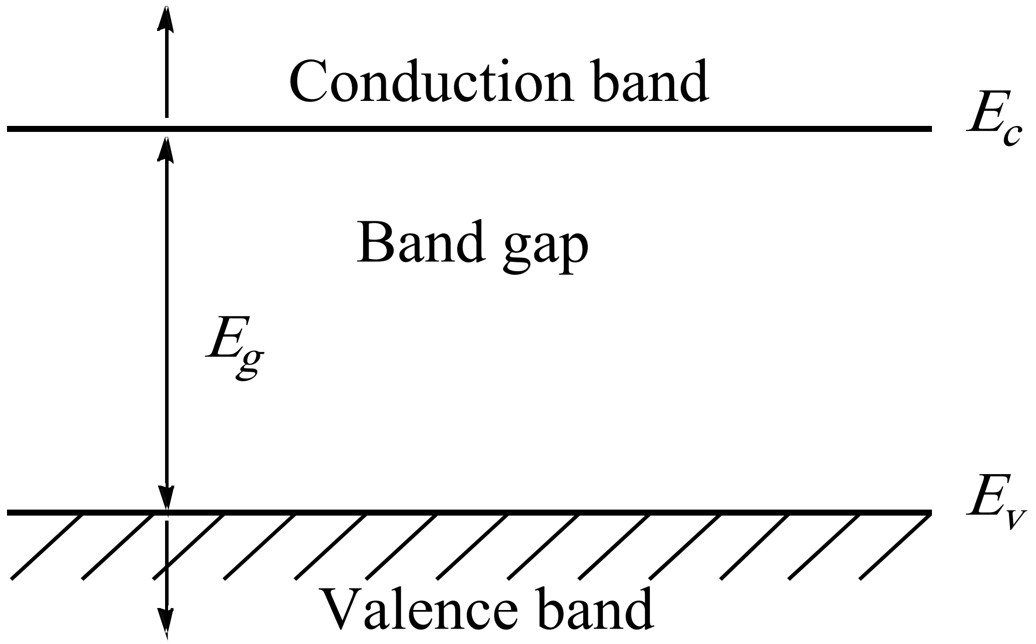
- Quantitatively, the formation of allowable energy bands separated by forbidden energy gaps arises from the solution of Schrodinger equation for a periodic Coulombic potential well with period *a* (lattice constant)
- In solid state electronics last year, you studied the Kronig-Penney model which solves the Schrodinger equation for a 1D periodic rectangular well
- Although simpler than reality, it showed that possible solutions (wavefunctions) are obtained within allowed bands that are separated by gaps where no analytical solution can be obtained





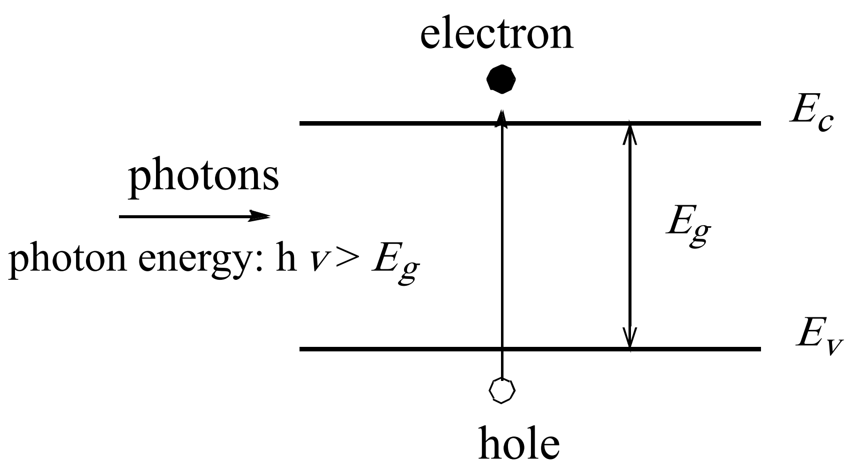
- In fact, <u>for any periodic potential well</u> (not necessarily rectangular), there will be discontinuities at $k = \pm n\pi/a$ and energy gaps will exist between allowed bands

Energy band diagram



- ***Valence band*** is the topmost filled energy band and **Conduction band** is the lowest empty energy band
- ***Energy band diagram*** shows the bottom edge of conduction band, E_c , and top edge of valence band, E_V .
- E_c and E_V are separated by the ***band gap energy***, $\boldsymbol{E_g}$.

Measuring energy gap by light absorption



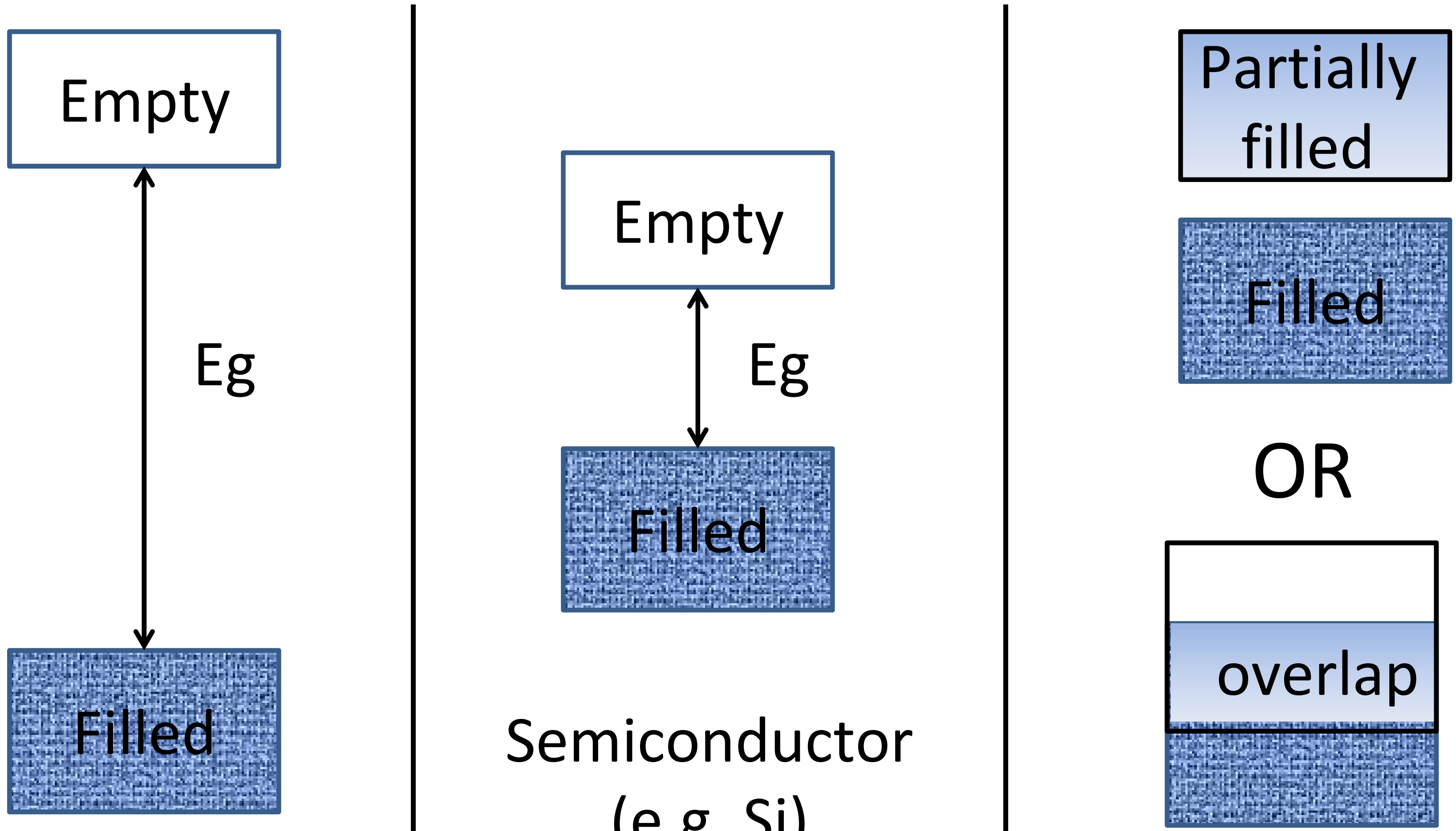
- E_g can be determined from the minimum energy ($h\nu$) of photons that are absorbed by the semiconductor.

Bandgap energies of selected semiconductors

Semi-conductor	InSb	Ge	Si	GaAs	GaP	ZnSe	Diamond
Eg (eV)	0.18	0.67	1.12	1.42	2.25	2.7	6

Distinction of metals, insulators and semiconductors

- **Totally filled and totally empty bands do not allow current flow**

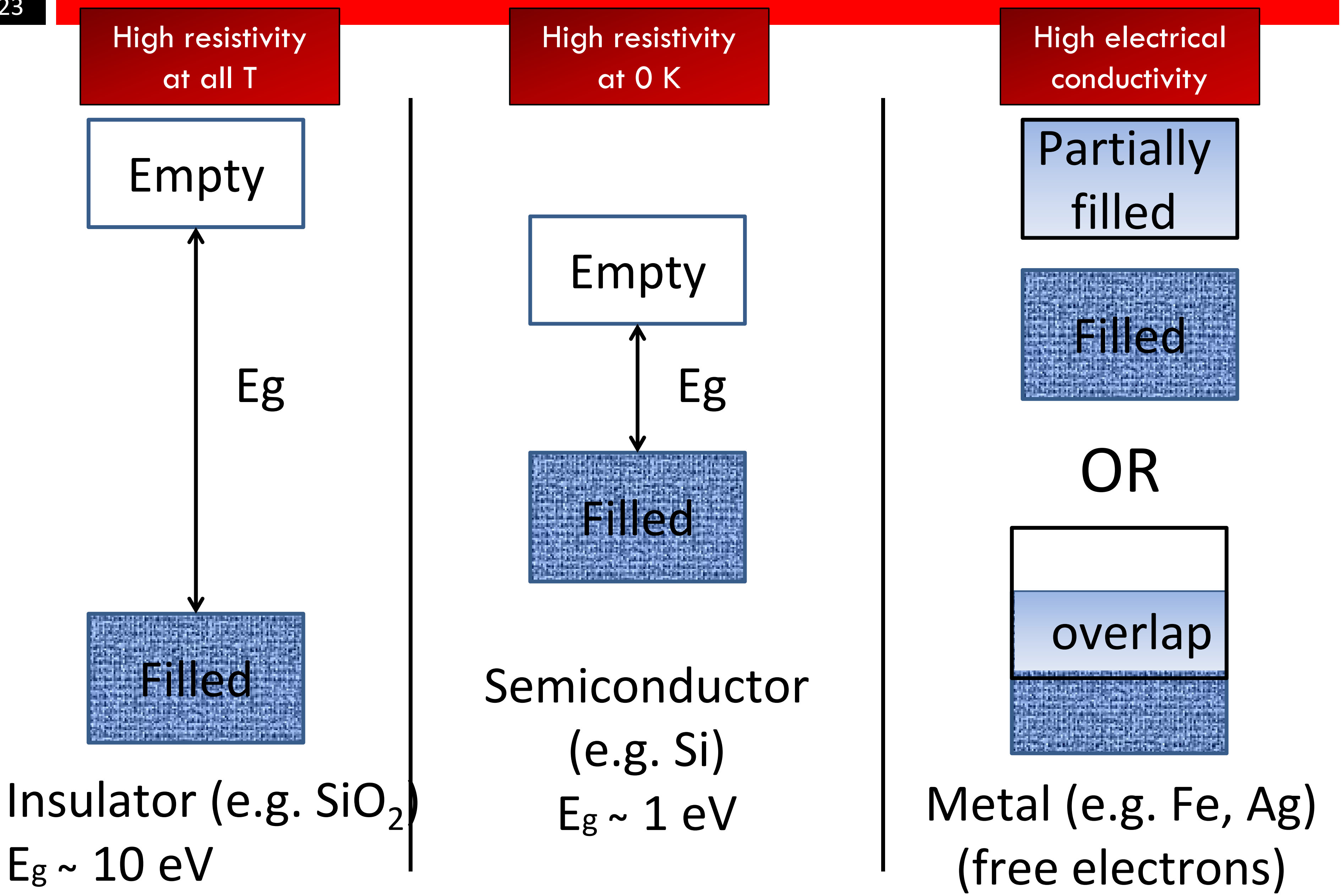


Insulator (e.g. SiO_2)
E_g ~ 10 eV

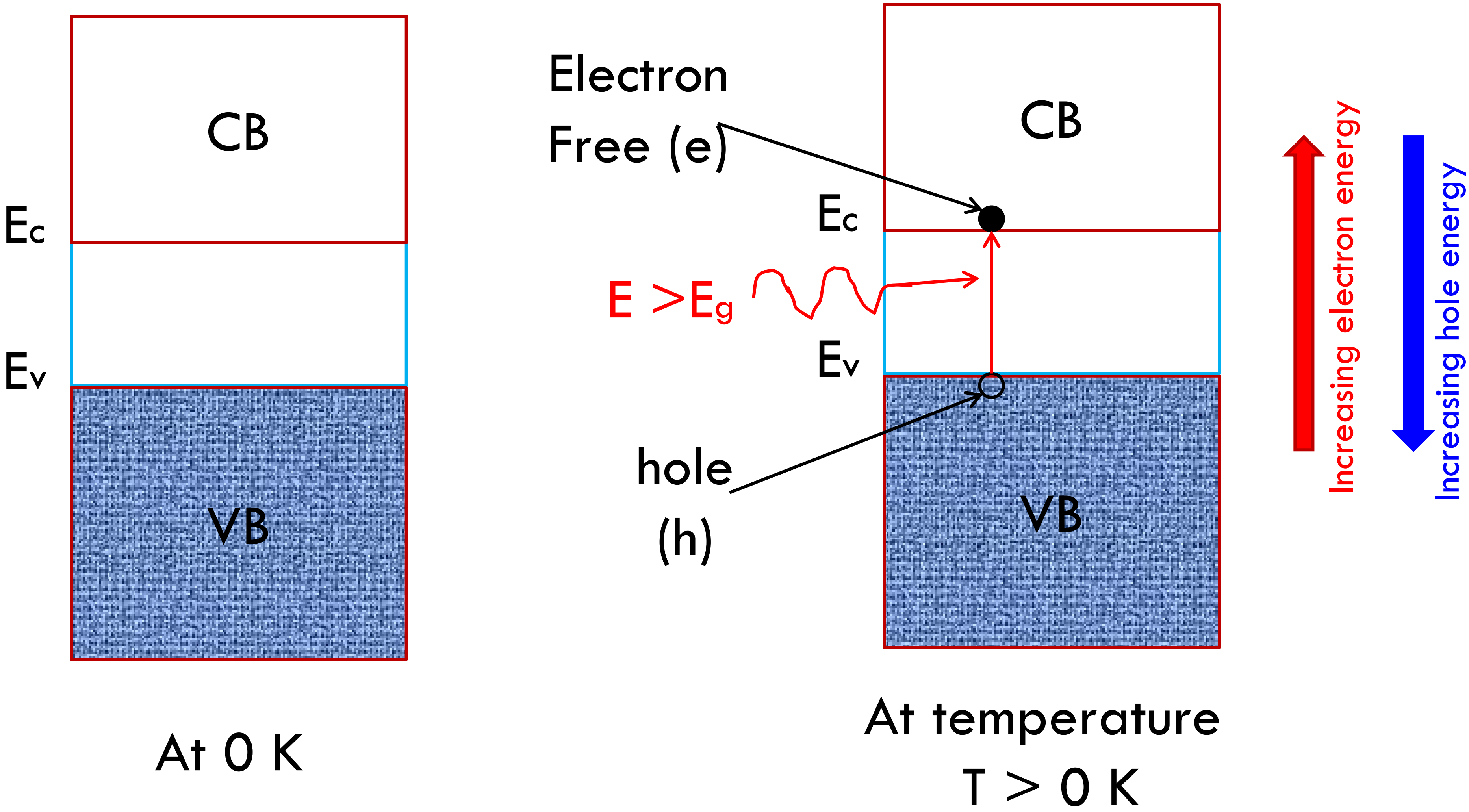
Semiconductor (e.g. Si)
E_g ~ 1 eV

Metal (e.g. Fe, Ag)
(free electrons)

Distinction of metals, insulators and semiconductors



Electron hole pair (EHP) generation



- Electrons and holes tend to fill their lowest possible energy level
- Electron hole pairs (EHPs) are the charge carriers and are responsible for current conduction