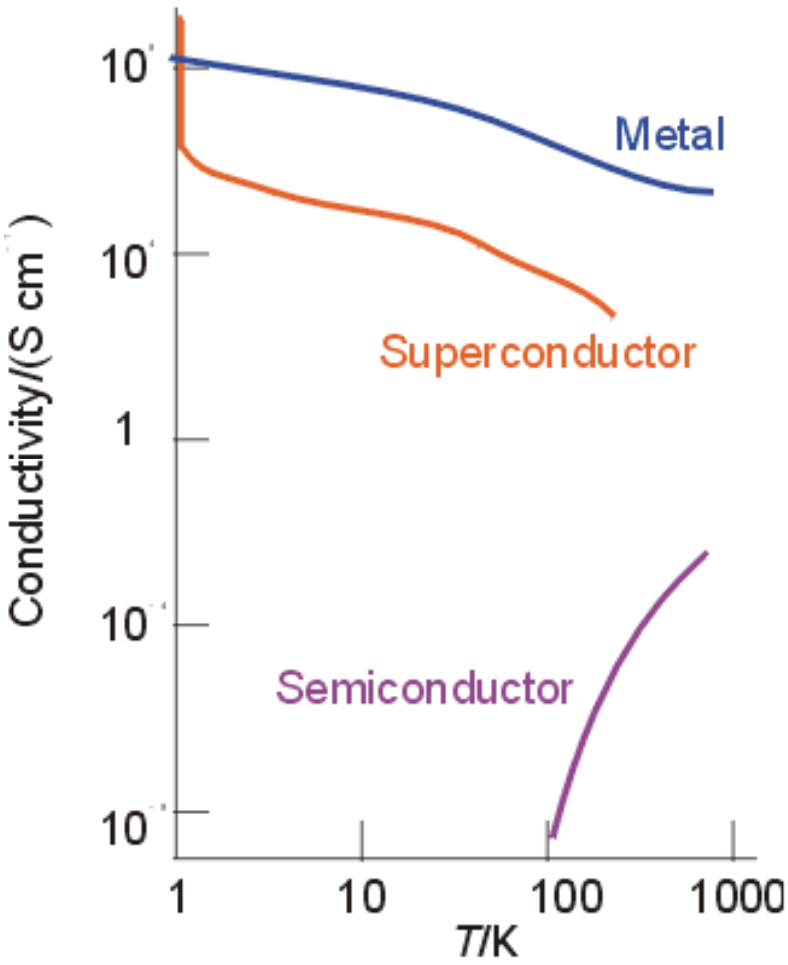
Molecular Orbital Theory of Solids

CHEM 245


Conductivity/(S cm⁻¹)
10²
10¹
1
10⁻¹
10⁻²
Metal
Superconductor
Semiconductor
1
10
100
1000
T/K

- **Metallic Conductor:** A substance with electrical conductivity which decreases with increasing T (increasing vibrational motion of the atoms interferes with the motion of the electrons and increases resistance to electron flow)

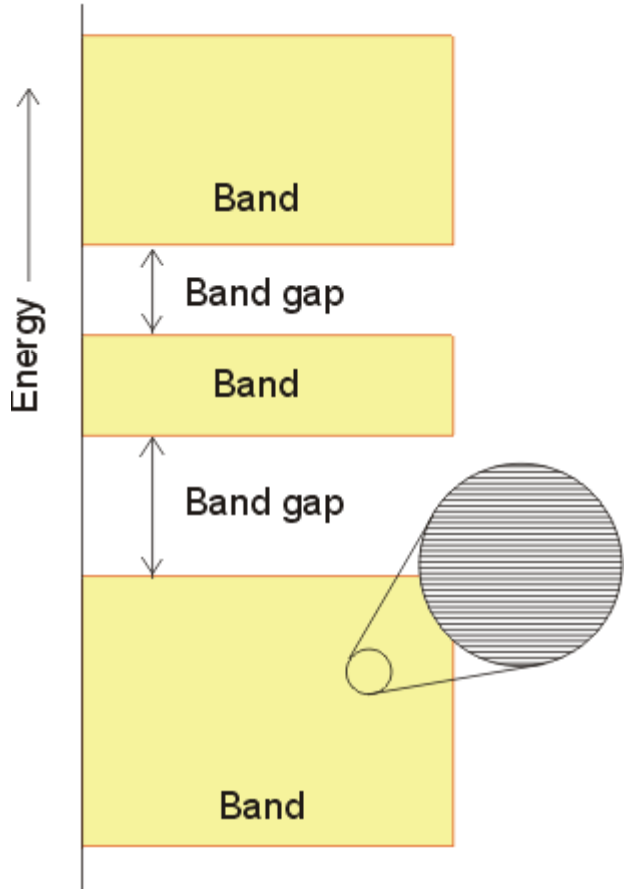
- **Semi-conductor:** A substance with electrical conductivity which increases with increasing T (with much higher conductivity than insulators and much lower conductivity than conductors)

- Conductivity of metals at R.T. > Conductivity of semi-conductors at R.T.

- **Solid Insulator:** Substance with very low electrical conductivity (However its conductivity also increases with increasing T)

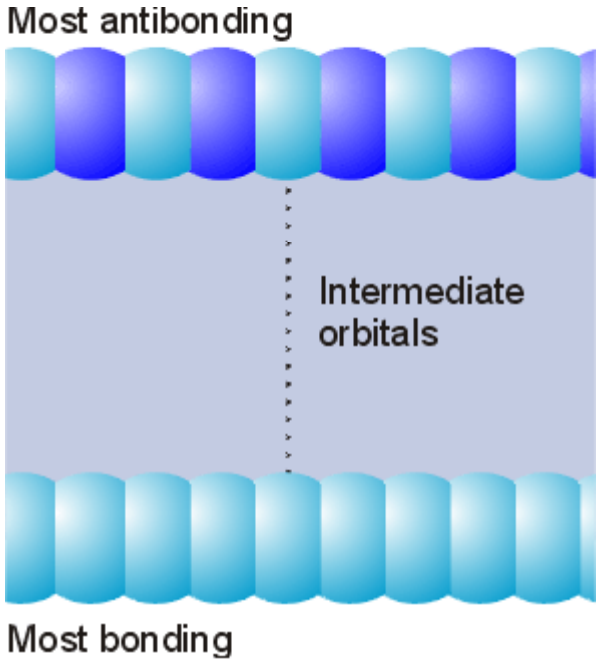
- **Superconductors:** Special class of materials that have zero electrical resistance below a critical T (10 K).

Molecular Orbital Bands



- When a very large number of atomic orbitals form molecular orbitals that are very close in energy, they form a virtually continuous **band**. Bands are separated by **band gaps**.

A node between every pair of neighbours



No nodes between neighbouring atoms

- N atomic orbitals ⟶ N molecular orbitals
- A band can be thought of as formed by bringing up atoms successively to form a line of atoms

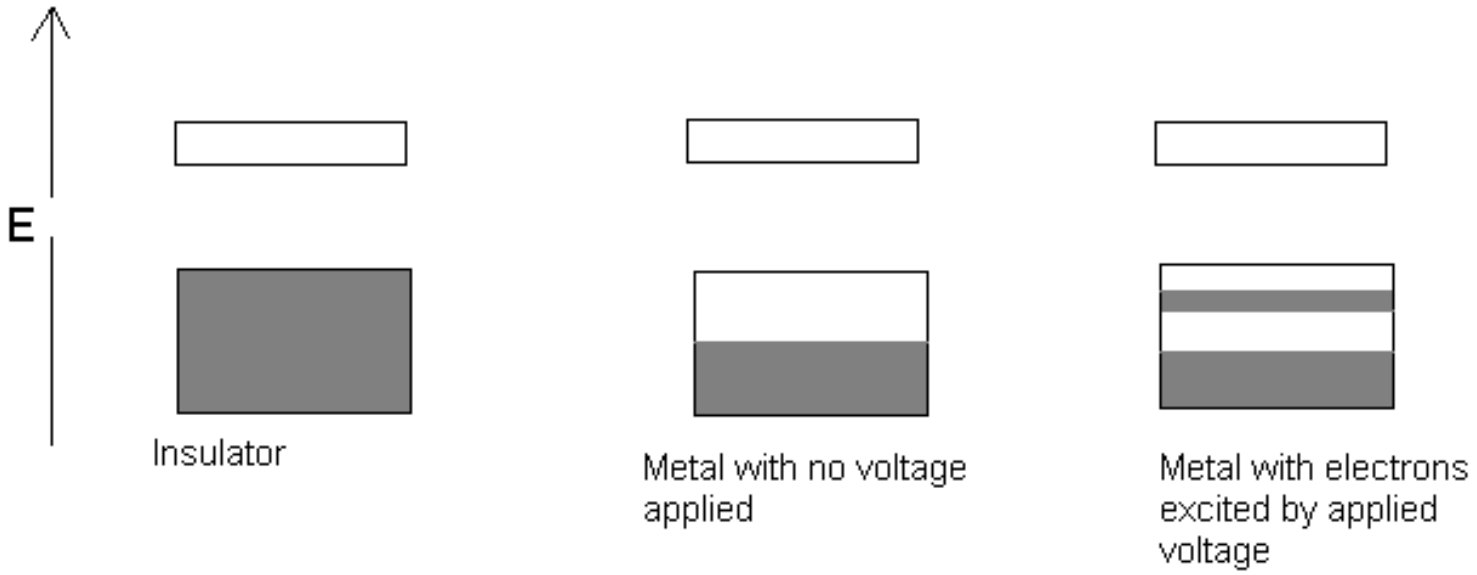
A band built from s-orbitals = **s band**

A band built from p-orbitals = **p band**

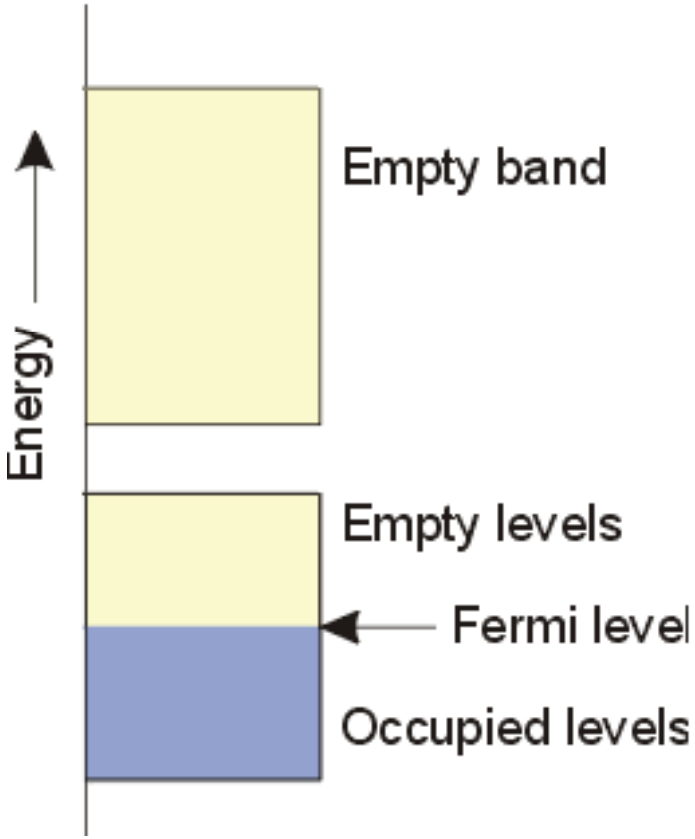
A band built from d-orbitals = **d band**

The highest energy band containing electrons = **VALENCE BAND**

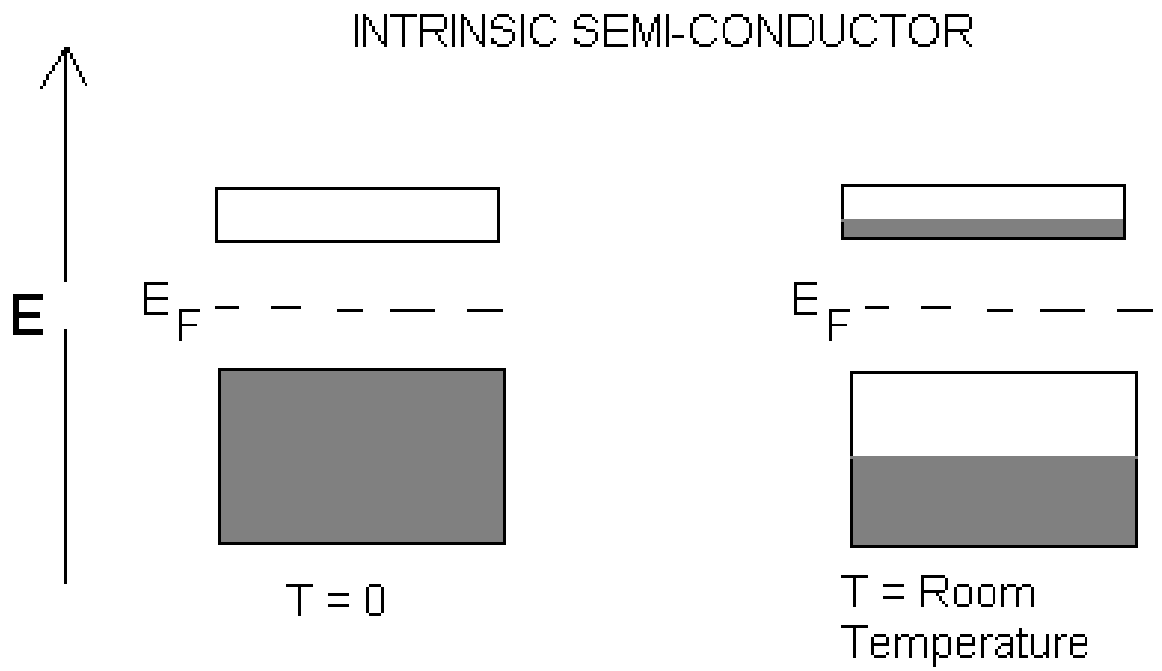
The next higher empty band = **CONDUCTION BAND**

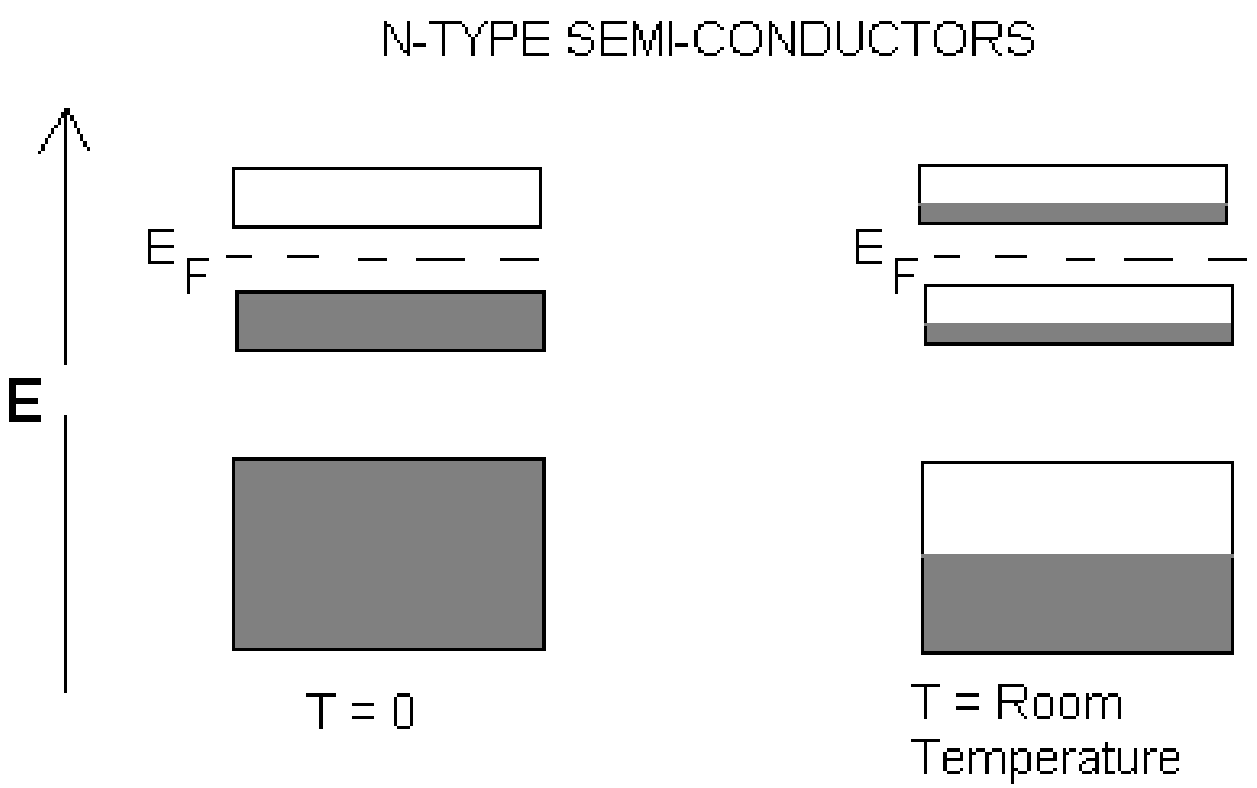


Semi-Conductors



In an intrinsic semi-conductor, the
FERMI LEVEL, the energy at which an electron
is equally likely to be in each of the two levels,
is near the middle of the band gap.


INTRINSIC SEMI-CONDUCTOR
E
E_F
E_F
T = 0
T = Room
Temperature


N-TYPE SEMI-CONDUCTORS
E
E F
E F
T = 0
T = Room
Temperature

P-TYPE SEMI-CONDUCTORS