

Solid State Chemistry.

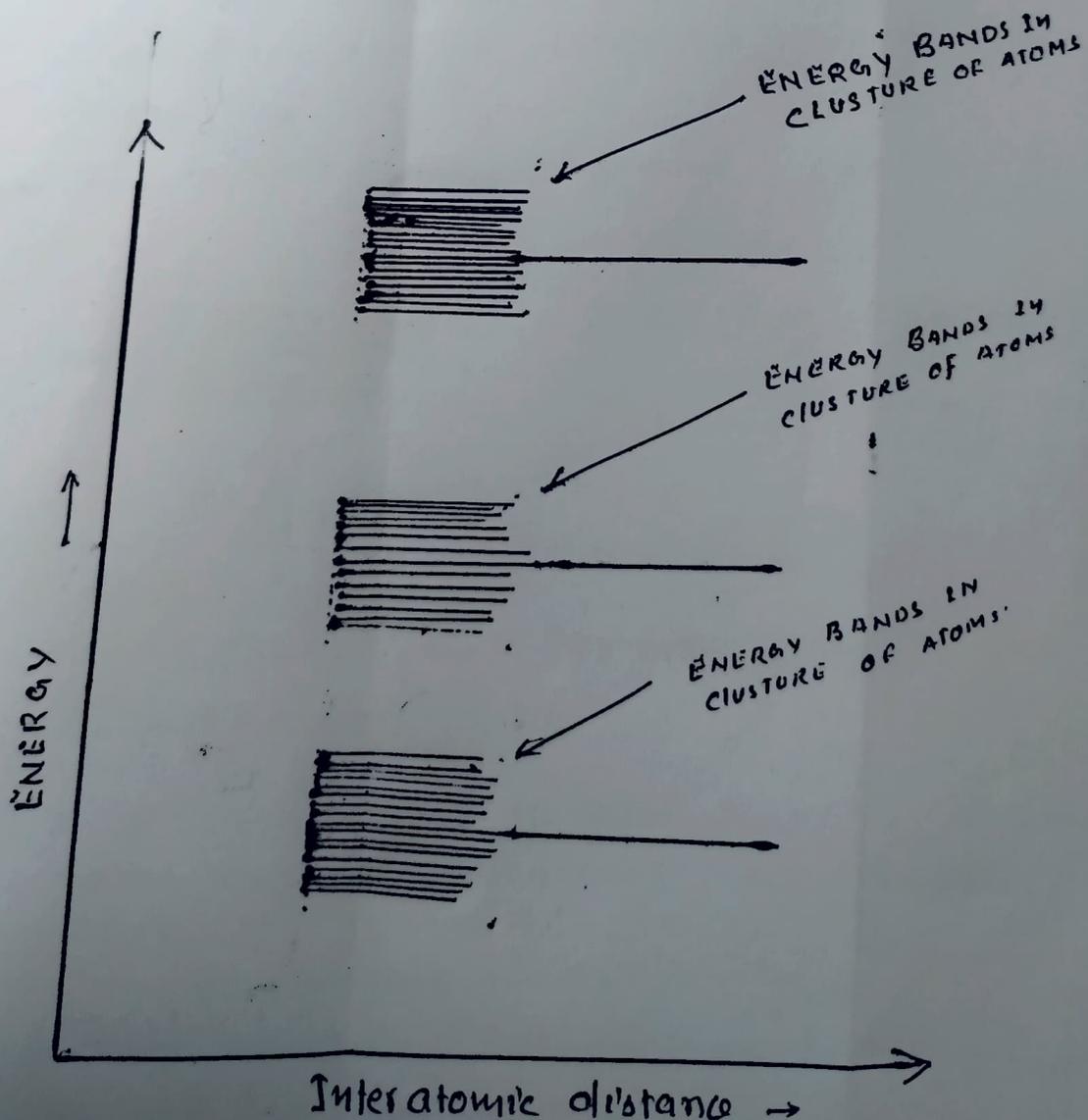
Role of Band theory of solids explain the behaviour of
Conductors,
Semi-Conductor
and Insulators.

The band theory of solids are able to explain the behaviour of Conductors, Semi-Conductors and insulators

The energy levels of electrons in an atom are quantised, but in a clusture of atoms, as in a metallic Solid, these energy levels become so closer that they constitute a band.

And it is obvious that the difference in energy between the energy levels within a band is very small or little as compared to the energy gaps between the band. It is obvious in the figure given below.

A graph is plotted between Energy & Interatomic distance.



Conductors: - A conductor is a material that allows the easy flow of electric charge or heat due to presence of free electron.

Such metals are refer as Conductor in which the valence band is full of electrons while the conduction band is only partly filled.

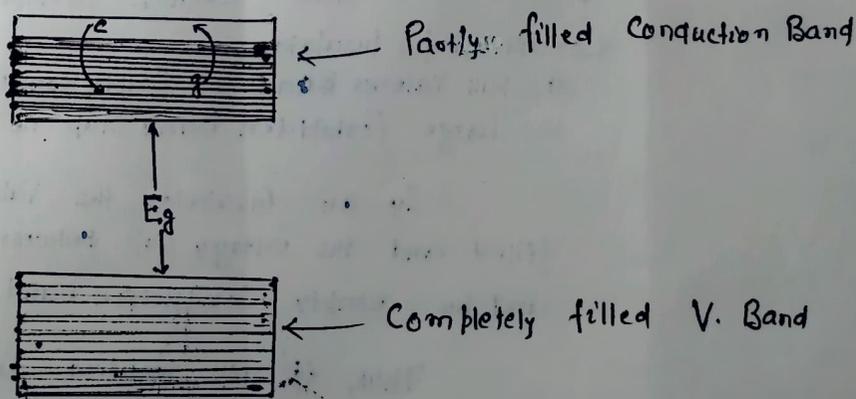
Only a small amount of energy is sufficient to allow the electrons to move within the conduction band therefore some rising to the higher energy level and other returning to a lower energy level.

This movement of electrons within the conduction band constitutes electrical conduction.

In some metallic conductors, the valence band and conduction band actually overlap resulting in a partly filled valence as well as conduction bands.

This difference in energy between the valence band and the conduction band is called Energy Gap or E_g .

In case of Conductor Energy bands is given below



Or, We can say according to band theory, a conductor is a material where the valence band and conduction band overlap. Or the valence band is partially filled, resulting in no forbidden energy gap ($E_g = 0$).

This structure provides a high density of free electrons movement and high electrical conductivity.

Characteristics of Conductors in Band theory: -

- (a) **Overlapping bands:** - The highest occupied energy band (valence band) and the lowest unoccupied energy band (conduction band) overlap.
- (b) **NO Band Gap:** - There is no forbidden energy gap between the valence band and conduction band.

Partially filled Band: -

In some cases, a single band is only partially filled, allowing electrons to move to higher energy states within that same band.

High Conductivity: -

High conductivity is due to abundance of free mobile electrons at all temperatures (even at absolute zero) these materials exhibit high conductivity.

Insulators

According to Band Theory (extension of MOT)

An insulator is defined by its electronic structure. Specifically the energy gap between the filled valence band and empty conduction band.

Condition for insulator: -

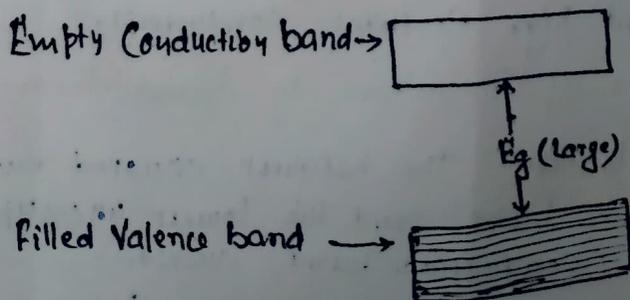
- (a) Full Valence Band
- (b) Empty Conduction Band
- (c) Large Forbidden Band Gap i.e. E_g .

In an insulator the valence band is completely filled and the energy gap between the valence band and the empty conduction band is very high.

Thus, it will require large amount of energy to make an electron jump the large energy gap and go to the conduction band.

This does not occur at very high temperature or under very high electric fields.

Energy band of an insulator is given below.



mi. Conductors: -

According to band theory. Semiconductor is a material with a small forbidden energy [E_g] gap between a completely filled valence band and an empty conduction band at 0K.

Due to this small gap, thermal energy at room temperature allows some electrons to gain enough energy to jump to the conduction band, so conductivity increases with temperature.

In an intrinsic semi-conductor, like Si and Ge, the valence band is full and conduction band is empty at very low temperature. The energy gap between valence and conduction bands, is so small that the electron can jump across it by the addition of a small thermal energy. The electrical conductivity increases with increase in temperature since more and more electrons are promoted from the valence band to the conduction band.

The smaller the value of E_g , the better is the semi-conductor. For Ge E_g value is 0.67 eV & "Si" E_g value is 1.14 eV. etc.

Whenever an electron jumps from the valence band to the conduction band, a positive hole is created in valence band.

An electron can move from another part of the valence band into the positive hole leaving a similar positive hole at its initial place.

Thus movement of positive hole is in operation in the valence band.

Conduction can occur either by the negatively charged electrons moving within the conduction band.

Energy bands of a semi-conductor can be represented as follows.

