Band Theory Of Metals

Explanation : Molecular orbital theory extended to solids is referred as Band Theory.

Example : Construction of a crystal of a sodium metal by adding Na atoms one at a time forming first Na_2 than Na_3, Na_4 ,Na_n respectively.

In Na_2 molecule, each Na-atom has electronic configuration [Ne] $3s^1$, with a single 3s valence electron. Two 3s-atom orbitals, one from each Na-atom, overlap to form two molecular orbitals σ (3s) and σ *(3s). There are just two valence electrons, which will occupy lower energy bonding molecular orbital σ (3s). The antibonding molecular orbital σ* (3s) is vacant.

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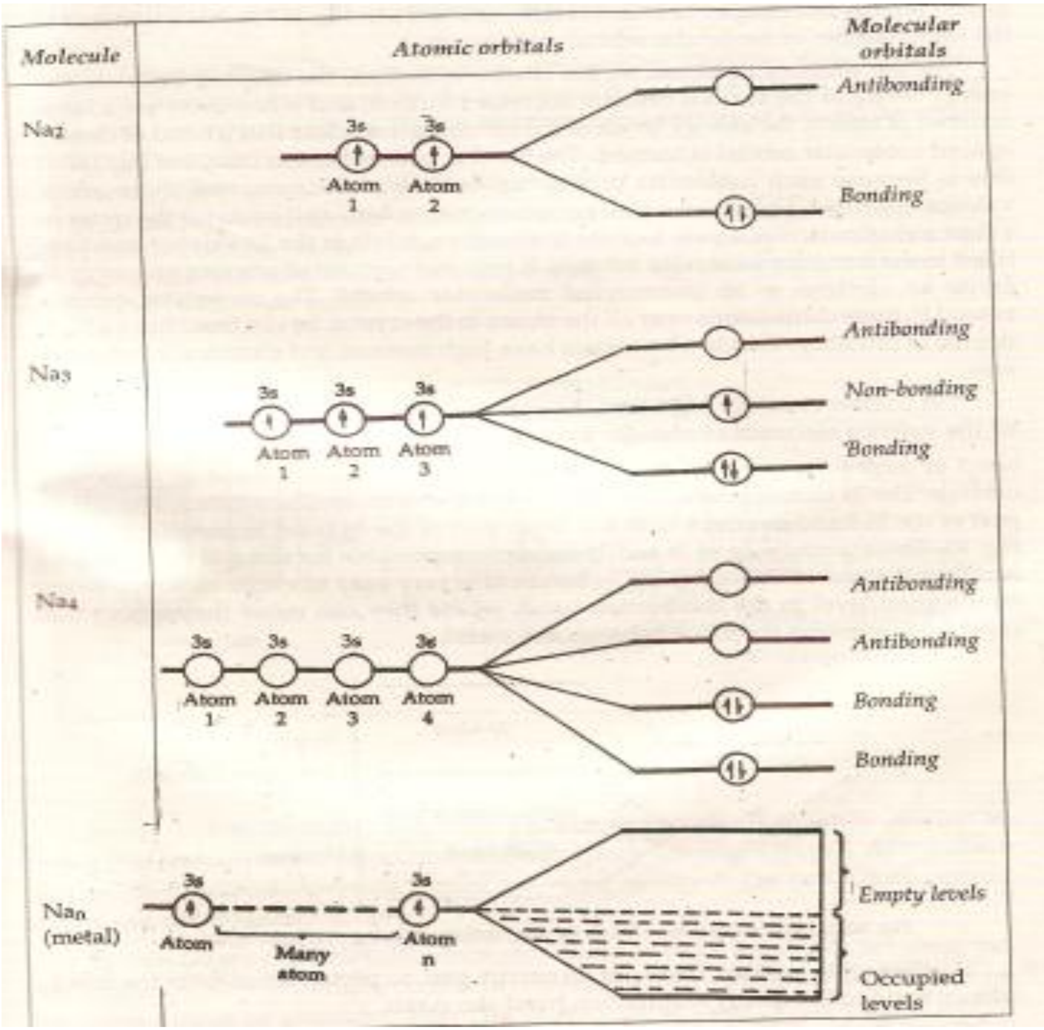

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Three Na atoms joined to form Na_3. Three 3s atomic orbitals would combine to form three molecular orbital one bonding, one non-bonding and one antibonding. The energy of the non-bonding MO is between that for the bonding and antibonding orbitals. The three valency electrons from the three sodium atoms would occupy the bonding and non-bonding molecular orbitals .

In Na_4, the four atomic orbitals would form four molecular orbitals-two bonding, and two anti-bonding. The four valence electrons would occupy the two lowest energy bonding molecular orbitals, half of the total number of molecular orbitals are vacant.

As the number of atoms in the cluster increases, the spacing between the energy levels of the various orbitals decreases further, and when there are a large number of

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atoms, the energy levels of the orbitals are so close that a band of closely spaced molecular orbital is formed. The band is half-full because each molecular orbital can hold two electrons, and there are N valence electrons. This band is also known as *valence band* as it contains the outer or valence electrons. The empty band is known as conduction band. Since only half the molecular orbitals in the 3s valence band are filled in the bonding molecular orbitals. It requires very small amount of energy to excite an electron to an unoccupied molecular orbital. The molecular orbitals extend in there dimensions over all the atoms in the crystal. So electrons have a high degree of mobility. That is why metals have high thermal and electrical conductivities.

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Explanation of Metallic Properties

(a) ***Electrical conduction :*** In metals, molecular orbitals extend in three dimen-sions over all the atoms and electrons have a high degree of mobility. In the absence of an electric field, equal number of electrons will move in all directions but in the presence of electric field, electrons readily move towards anode and hence electric current flows.

(b) ***Thermal conduction:*** The mobile electrons gain energy from the heated end and move to an unoccupied molecular orbital where they can travel rapidly to colder part of the metal. Thus, mobile electrons account for the high thermal conduction of metals.

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(c) ***Effect of Temperature on electrical conductivity :*** The free flow of mobile valence electrons is obstructed by the increased thermal vibrations of the metal atoms with rise in temperature. Hence, electrical conductivity of a metal decreases with rise in temperature.

Usefulness of band Theory Of Metals

With the help of Band theory, we can classify materials into three categories viz. conductors, insulators and semi-conductors, depending on the energy gap between the valence and conduction bands.

In conductors (metallic), either the valence and conduction bands overlap or the valence band is only partly full .

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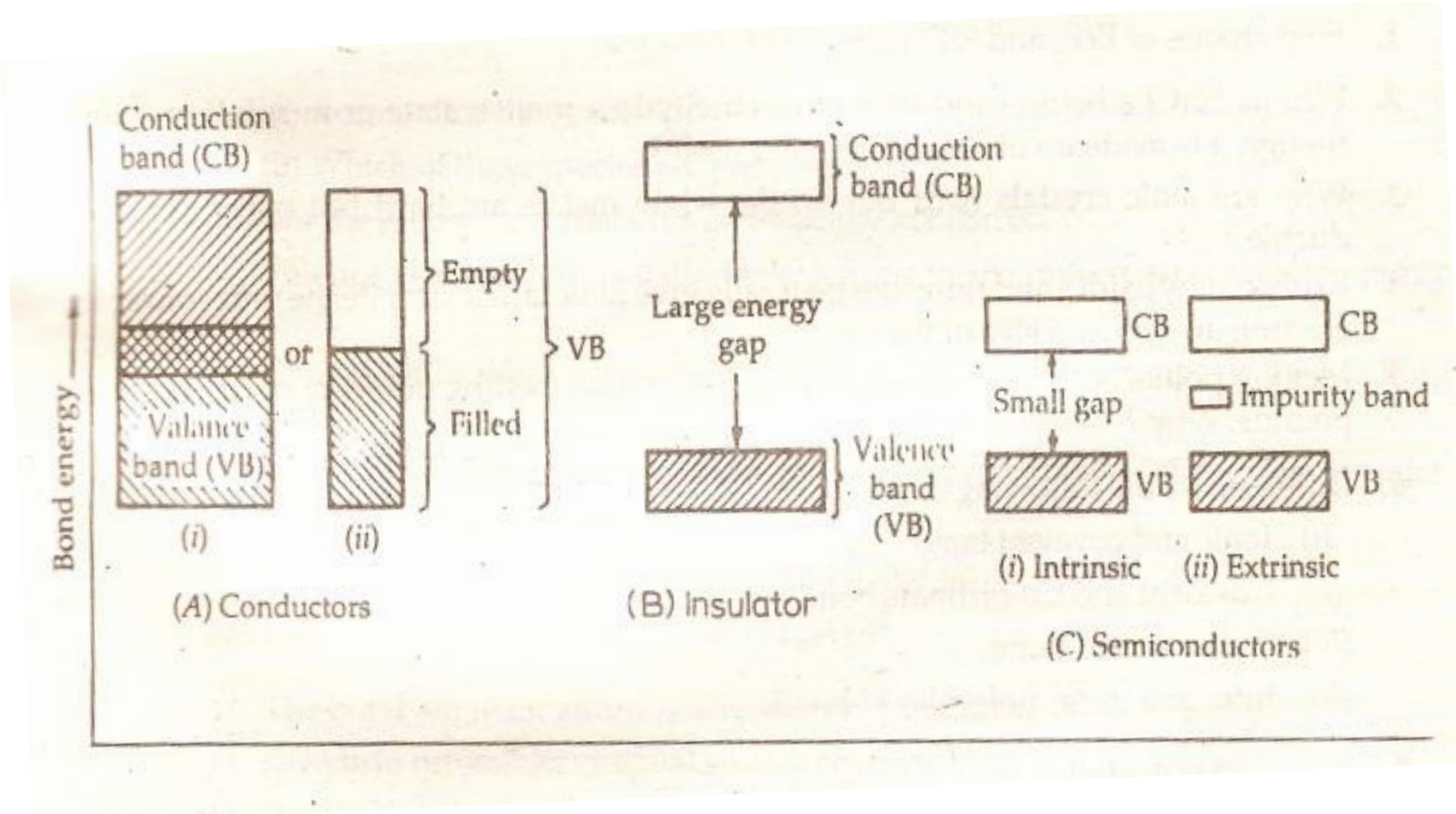

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In Insulators (non-metallic elements), there is large band gap between the filled valence band and empty conduction band as in diamond. Therefore Electrons cannot qe promoted from the valence band to conduction band where they could move freely.

Semiconductors are of the types, intrinsic and extrinsic semiconductors. Intrinsic semiconductors (like Si or Ge) are having small energy gap between the filled valence band (VB) and empty conduction band (CB) sufficient to promote an electron from VB to CB. The hole left in the VB and the promoted electron in the CB both contribute towards conductivity.

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The number of electrons promoted to CB increases with rise in temperature, thus conductivity of semiconductors increases with temperature. The conductance of semiconductors can also be improved by doping. Doping means treatment of Si and Ge with impurity atoms of Gp. (III) and Gp (v) giving respectively *p-type* and n-type semiconductors. Basically the band from the impurity lies in between the VB and CB , so that electrons may easily excited from VB to impurity band and hence conductance increases.