

What is the significance of Electron Band Gap?

The concept of electron band gap pertains to solid state chemistry. This is a schematic way of visualizing the electronic configuration in outermost shells. The concept helps in understanding characteristics of metals (conductors), semiconductors and insulators (non-metals). It is the electrons in the outer shells that decide most of the properties of matter. Mobility of these electrons across the matter governs their intrinsic properties like conductivity and absorption of light. To understand the movement of the electrons in the outer shell, the concept of electron bands is very important. There are two types of electron bands:

Valence band: This is the band or space or orbitals that are outermost in the electronic configuration of atoms (or molecules). The probability of finding outermost electrons in this region is the highest. These are also called as Highest Occupied Molecular Orbital or HUMO. These represent the ground state or unexcited energy level of the material. The electrons in this valence band are attached to the nucleus and are not mobile unless they move into the conduction band.

Conduction band: This is a higher energy level discretely separated from the valence band. It represents an orbital or space into which electrons from the valence band can be transferred upon excitation. Normally, the conduction band does not contain electrons and hence are also called as Lowest Unoccupied Molecular Orbital or LUMO. Once the electrons are in the conduction band, they can travel freely across atoms (or molecules) throughout the piece of matter and conduct electricity.

Figure below is a schematic representation of the concept of electron band gap.

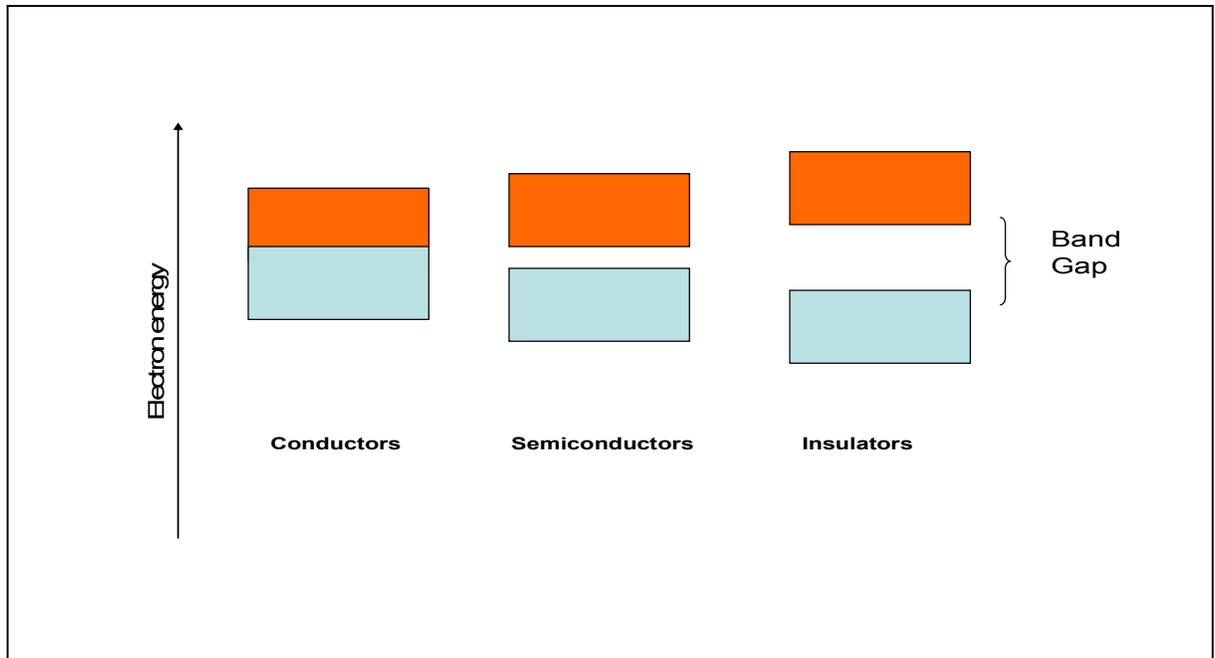


Figure: Band structure of matter

According to quantum mechanics, the energy levels in atoms or molecules are not continuous, but discrete. Hence there is a well defined gap between the valence band and the conduction band. This is called as the 'electron band gap' and is an important concept to understand many phenomena associated with the nanomaterials. The band gap is expressed in terms of electron volts (eV) which is a very small unit signifying the energy acquired by an electron accelerated across the potential difference of 1 volt.

The larger the band gap, the greater the difficulty for the valence electrons to jump to the conduction band. This explains poor electrical conductivity of non-metals (insulators). Whenever there is an overlap of valence and conduction bands, the electrons can move across freely into the conduction band as happens in the case of metals (conductors). If the band gap is narrow, the electrons can be elevated to the conduction band with small amount of energy. Such materials are semiconductors.

The concept of band gap is also useful in understanding the interaction of light with matter. The band gap is a useful predictor of wavelength of light that will be absorbed by the material. This

relationship is inverse. The narrow band gap materials can absorb in the high wave length visible range due to lower energy requirement for transition of the electron into the conduction band. The large band gap materials absorb in the short wavelength UV region due to the high energy required by the valence electrons to jump across a wide gap to the conduction band. The semiconductors have a very narrow band gap of 1~3 eV and these generally absorb in the near UV region (UV A&B).

Band gap is the intrinsic property of the material. However, in the nanoscale region there is an alteration in the band gap and the dependant properties.
