

**DEPARTMENT OF PHYSICS AND NANOTECHNOLOGY  
SRM INSTITUTE OF SCIENCE AND TECHNOLOGY**

**ENERGY BAND STRUCTURE OF  
SEMICONDUCTOR & CONCEPTS OF EFFECTIVE  
MASS**



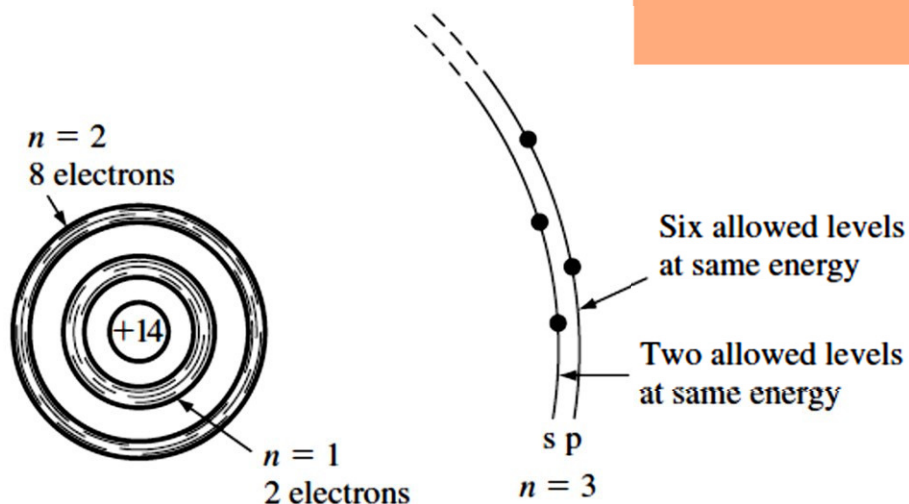
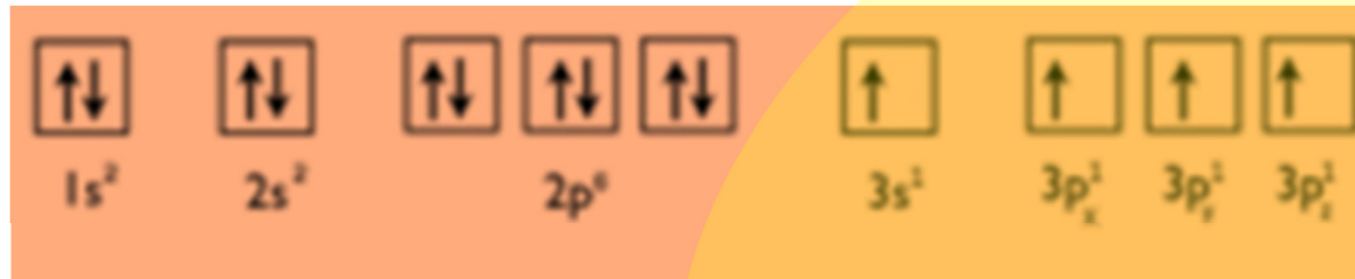
# Energy Band Structure of Semiconductor Brillouin zone



To understand the Energy band structure, consider silicon atom. A schematic representation of an isolated silicon atom is shown in Figure.

Ten of the 14 silicon atom electrons occupy deep-lying energy levels close to the nucleus. The four remaining valence electrons are relatively weakly bound and are the electrons involved in chemical reactions.

$1s^2, 2s^2 2p^6, 3s^2 3p^2$

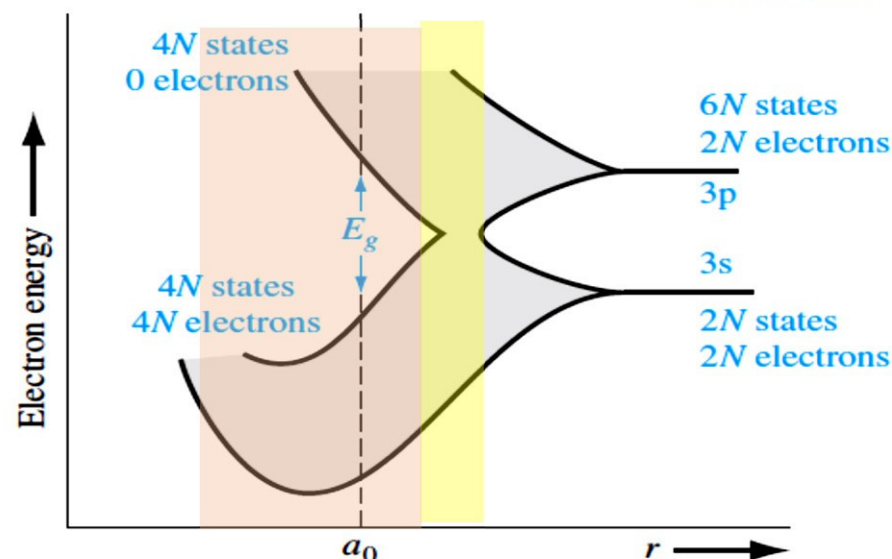
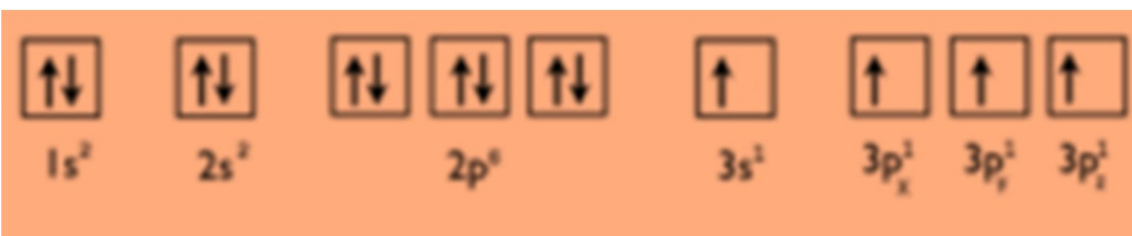




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$1s^2, 2s^2 2p^6, 3s^2 3p^2$



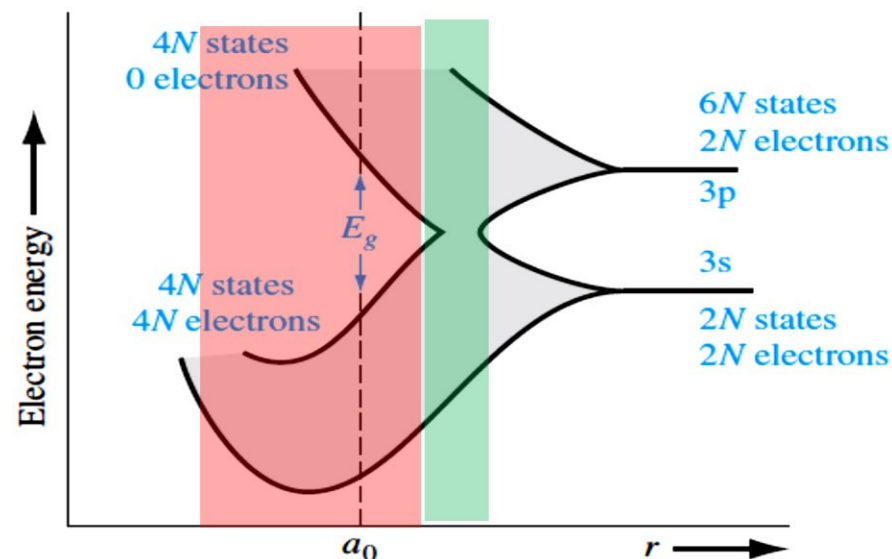
Above Figure shows the **band splitting of silicon**. We need only to consider the  **$n=3$  level** for the valence electrons, since the **first two energy shells are completely full and are tightly bound to the nucleus**.

The  **$3s$  state** corresponds to  $n=3$  and  $l=0$  and contains two quantum states per atom. This state will contain two electrons at  $T=0$  K. The  **$3p$  state** corresponds to  $n=3$  and  $l=1$  and contains six quantum states per atom. **This state will contain the remaining two electrons in the individual silicon atom.**

# Energy Band Structure of Semiconductor Brillouin zone



As the interatomic distance decreases, the 3s and 3p states interact and overlap (*covalent bonding and crystal formation*).



- At the **equilibrium** interatomic distance, the bands have again split, but now four quantum states per atom are in the lower band and four quantum states per atom are in the upper band.
- At 0 K, electrons are in the lowest energy state, so that all states in the lower band (the valence band) will be full and all states in the upper band (the conduction band) will be empty.
- The **bandgap energy**  $E_g$  between the top of the valence band and the bottom of the conduction band is the width of the forbidden energy band.



# Energy Band Structure of Semiconductor Brillouin zone



- At  $T = 0$  K, the  $4N$  states in the lower band, the valence band, are filled with the valence electrons. All of the valence electrons are in the valence band. The upper energy band, the conduction band, is completely empty at  $T = 0$  K.
- As the temperature increases above 0 K, a few valence band electrons may gain enough thermal energy to break the covalent bond and jump into the conduction band.
- This means that, as the negatively charged electron breaks away from its covalent bonding position, a positively charged “empty state” is created in the original covalent bonding position in the valence band.
- **As the temperature further increases, more covalent bonds are broken**, more electrons jump to the conduction band, and more positive “empty states” are created in the valence band.

For 1 eV

$$E = k_b T$$

$$\Rightarrow T = E / k_b = \frac{1.6 \times 10^{-19} \text{ Jule}}{1.38 \times 10^{-23} \text{ m}^2 \text{ Kg s}^{-2} \text{ K}^{-1}}$$

$$\Rightarrow T = \frac{1.6 \times 10^{23} \times 10^{-19}}{1.38} \text{ K}$$

$$= \frac{1.6 \times 10^4}{1.38} \text{ K} = \frac{16000}{1.38} \text{ K}$$

$$= 11,594.2 \text{ K}$$

$$\approx 11.5 \text{ Thousand K}$$

$$\approx 10^4 \text{ K}$$

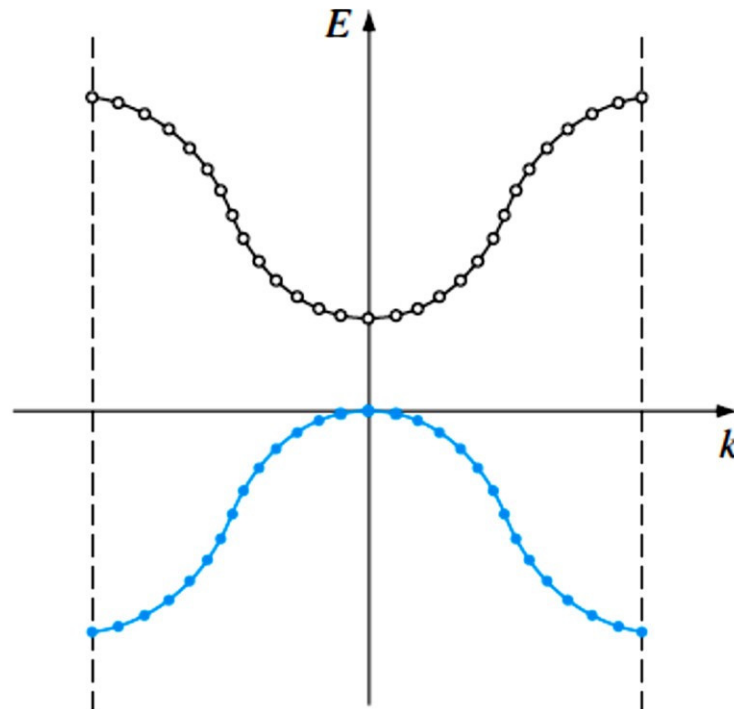


# Energy Band Structure of Semiconductor Brillouin zone



This bond breaking can be related to the  $E$  versus  $k$  energy bands (first Brillouin zone).

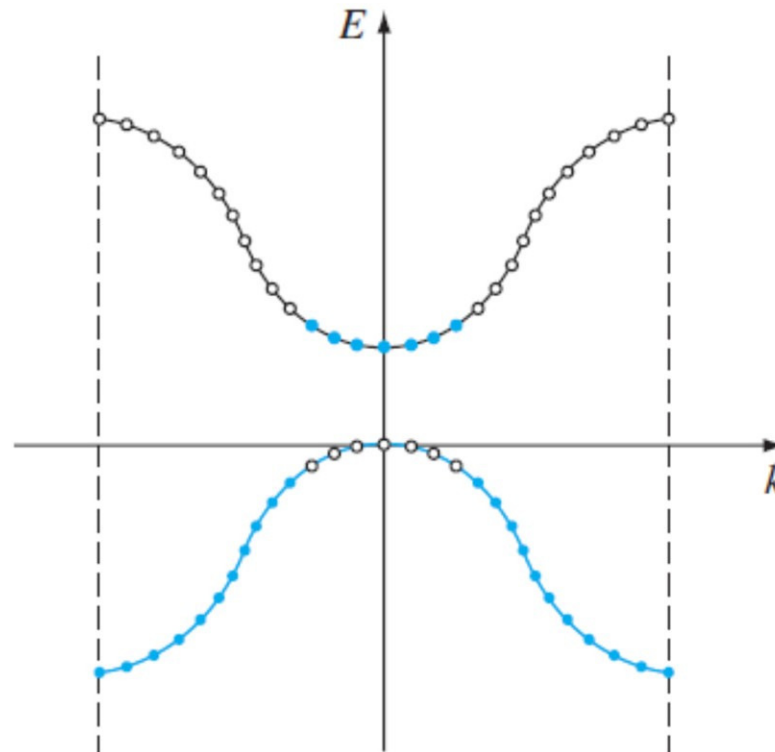
Figure shows the  $E$  versus  $k$  diagram of the **conduction and valence bands at  $T=0$  K**. The energy states in the valence band are completely full and the states in the conduction band are empty.



# Energy Band Structure of Semiconductor Brillouin zone



Below Figure shows **the same bands for  $T > 0$  K**, in which some electrons have gained enough energy to jump to the conduction band and have left empty states in the valence band.



**The movement of an electron in a lattice will**, in general, be different from that of an electron in free space.

In addition to an externally applied force, there are internal forces in the crystal due to positively charged ions or protons and negatively charged electrons, which will influence the motion of electrons in the lattice.

Then

$$F_{total} = F_{ext} + F_{int} = ma \quad (1)$$

where  $F_{total}$ ,  $F_{ext}$ , and  $F_{int}$  are the total force, the externally applied force, and the internal forces, respectively, acting on a particle in a crystal. The parameter  $a$  is the acceleration and  $m$  is the rest mass of the particle.



Since it is difficult to take into account all of the internal forces, the equation becomes

$$F_{ext} = m^*a \quad (2)$$

where the acceleration  $a$  is now directly related to the external force. The parameter  $m^*$ , *called the effective mass, takes into account the particle mass and also takes into account the effect of the internal forces.*

To use an analogy for the effective mass concept, consider the difference in motion between a **glass marble in a container filled with water** and **in a container filled with oil**. In general, the marble will drop through the water at a faster rate than through the oil. The **external force** in this example is the **gravitational force** and the **internal forces** are related to the **viscosity of the liquids**. Because of the difference in motion of the marble in these two cases, the mass of the marble would appear to be different in water than in oil.

The effective mass of an electron in a crystal can be related to the E versus k curves. E-k curves of semiconductor material contains allowed energy bands that are almost empty of electrons and other energy bands that are almost full of electrons.

Recalling Equation, the energy and momentum are related by

$$E = p^2/2m = \hbar^2 k^2/2m \quad (3)$$

where m is the mass of the electron. The momentum p and wave number k are related by  $p = \hbar k$ . Taking the derivative of Equation (3) with respect to k,

$$dE/dk = \hbar^2 k/m = \hbar p/m \quad (4)$$

Relating momentum to velocity, Equation (4) can be written as

$$(1/\hbar)(dE/dk) = p/m = v \quad (5)$$

where v is the velocity of the particle. The first derivative of E with respect to k is related to the velocity of the particle.

If we now take the second derivative of  $E$  with respect to  $k$ , we have

$$d^2E/dk^2 = \hbar^2/m \quad (6)$$

Equation (6) can be rewritten as

$$(1/\hbar^2)d^2E/dk^2 = 1/m^* \quad (7)$$

The second derivative of  $E$  with respect to  $k$  is inversely proportional to the mass of the particle. For the case of a free electron, the mass is a constant (non relativistic effect), so the second derivative function is a constant.

If we apply an electric field to the free electron and use Newton's classical equation of motion, then

$$F_{ext} = m^* a = eE \quad (8)$$

where  $a$  is the acceleration,  $E$  is the applied electric field, and  $e$  is the magnitude of the electronic charge.

The effective mass is a parameter that relates the quantum mechanical results to the classical force equations.

In most instances, the electron in the bottom of the conduction band can be thought of as a classical particle whose motion can be modeled by Newtonian mechanics, provided that the internal forces and quantum mechanical properties are taken into account through the effective mass.

If we apply an electric field to the electron in the bottom of the allowed energy band, then the acceleration is

$$a = eE/m^* \quad (9)$$

$$m^* = \hbar^2 \cdot \frac{1}{\partial^2 E_n / \partial k^2 |_{k_{ex}}}$$

where  $m^*$  is the effective mass of the electron.