



جلسه ۵

# Energy Bands and Carrier Concentration in Thermal Equilibrium

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## ➤ 1.4 ENERGY BANDS

### 1.4.1 Energy Levels of Isolated Atoms

- For an isolated atom, the electrons can have discrete energy levels. For example, the energy levels for an isolated hydrogen atom are given by the Bohr model:

$$E_H = -m_0 q^4 / 8\varepsilon_0^2 h^2 n^2 = -13.6 / n^2 \text{ eV}, \quad (2)$$

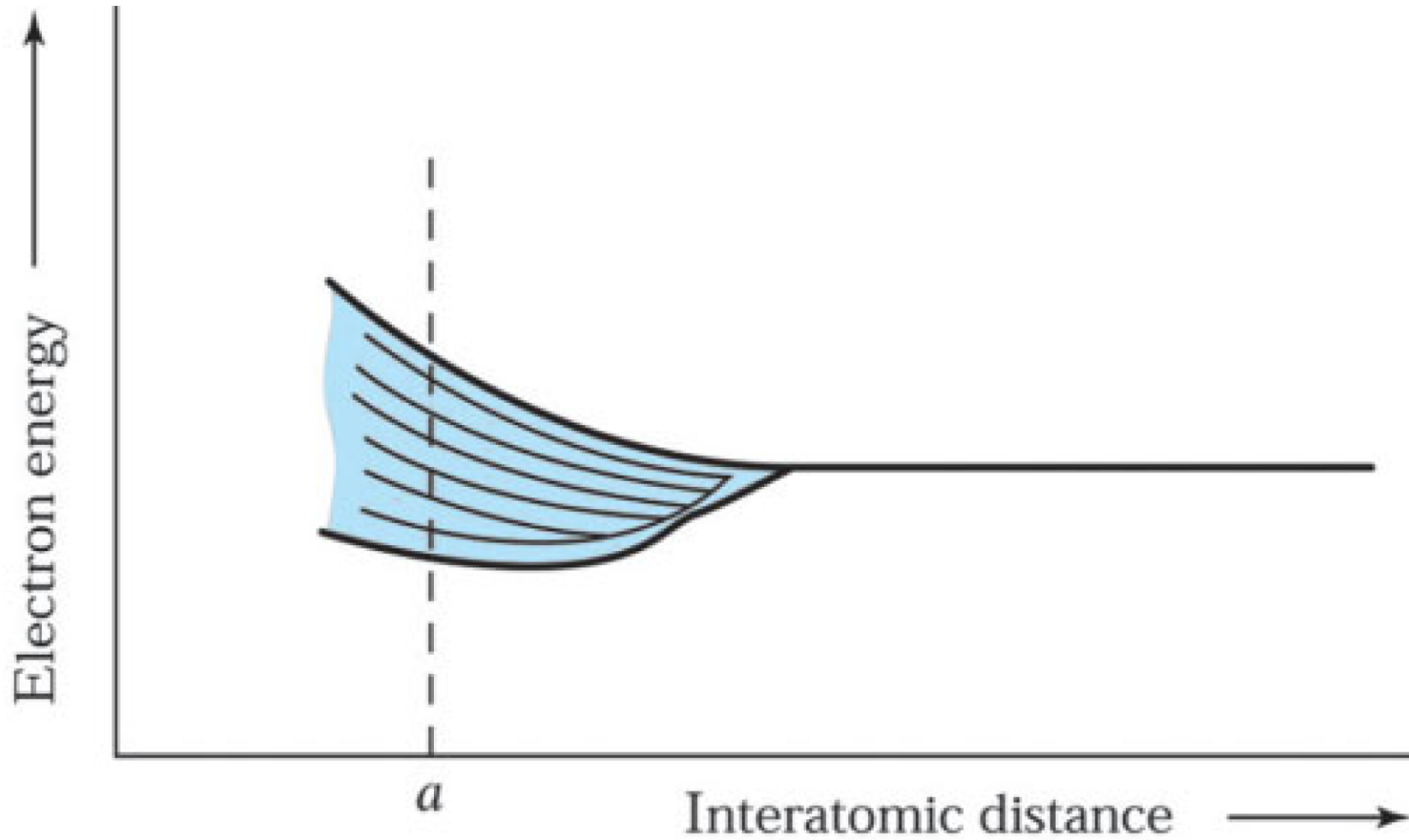
where  $m_0$  is the free-electron mass,  $q$  is the electronic charge,  $\varepsilon_0$  is the free-space permittivity,  $h$  is the Planck constant, and  $n$  is a positive integer called the principal quantum number.

The quantity eV (electron volt) is an energy unit corresponding to the energy gained by an electron when its potential is increased by one volt. It is equal to the product of  $q$  ( $1.6 \times 10^{-19}$  coulomb) and one volt, or  $1.6 \times 10^{-19}$  J. The discrete energies are  $-13.6$  eV for the ground-state energy level ( $n = 1$ ),  $-3.4$  eV for the first excited-state energy level ( $n = 2$ ), and so on. Detailed studies reveal that for higher principle quantum numbers ( $n \geq 2$ ), energy levels are split according to their angular momentum quantum number ( $\ell = 0, 1, 2, \dots, n - 1$ ).

- We now consider two identical atoms.
- When they are far apart, the allowed energy levels for a given principal quantum number (e.g.,  $n = 1$ ) consist of one doubly degenerate level; that is, both atoms have exactly the same energy.
- When they are brought closer, the doubly degenerate energy levels will split into two levels by the interaction between the atoms.
- The split occurs due to the Pauli exclusion principle, which states that no more than two electrons in a given system can reside (واقع شدن) in the same energy state at the same time.

- As  $N$  isolated atoms are brought together to form a solid, the orbits of the outer electrons of different atoms overlap and interact with each other.
- This interaction, including those forces of attraction and repulsion between atoms, causes a shift in the energy levels, as in the case of two interacting atoms. However, instead of two levels,  $N$  separate but closely spaced levels are formed.
- When  $N$  is large, the result is an essentially continuous band of energy. This band of  $N$  levels can extend over a few eV at the inter-atomic distance of the crystal.

- The electrons can no longer be treated as belonging to their parent atoms. They belong to the crystal as a whole.
- Figure 9 shows the effect, where the parameter  $a$  represents the equilibrium inter-atomic distance of the crystal.



**Fig. 9** The splitting of a degenerate state into a band of allowed energies.



- The actual band splitting in a semiconductor is much more complicated.
- Figure 10 shows an isolated silicon atom that has 14 electrons.
- Of the 14 electrons, 10 occupy deep-lying energy levels whose orbital radius is much smaller than the interatomic separation in the crystal.
- The four remaining valence electrons are relatively weakly bound and can be involved in chemical reactions.
- Therefore, we only need to consider the outer shell (the  $n = 3$  level) for the valence electrons, since the two inner shells are completely full and tightly bound to the nucleus. 9

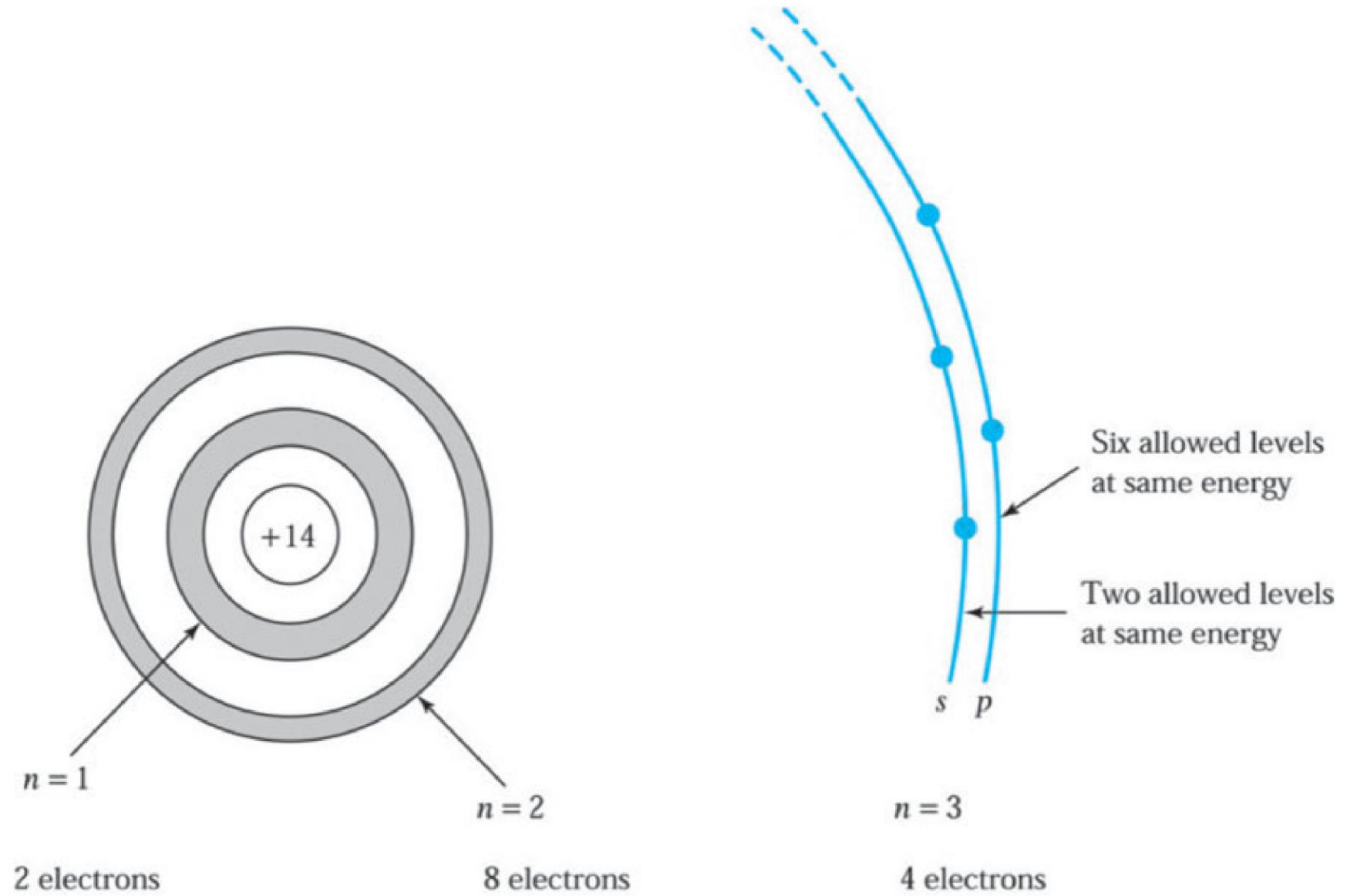
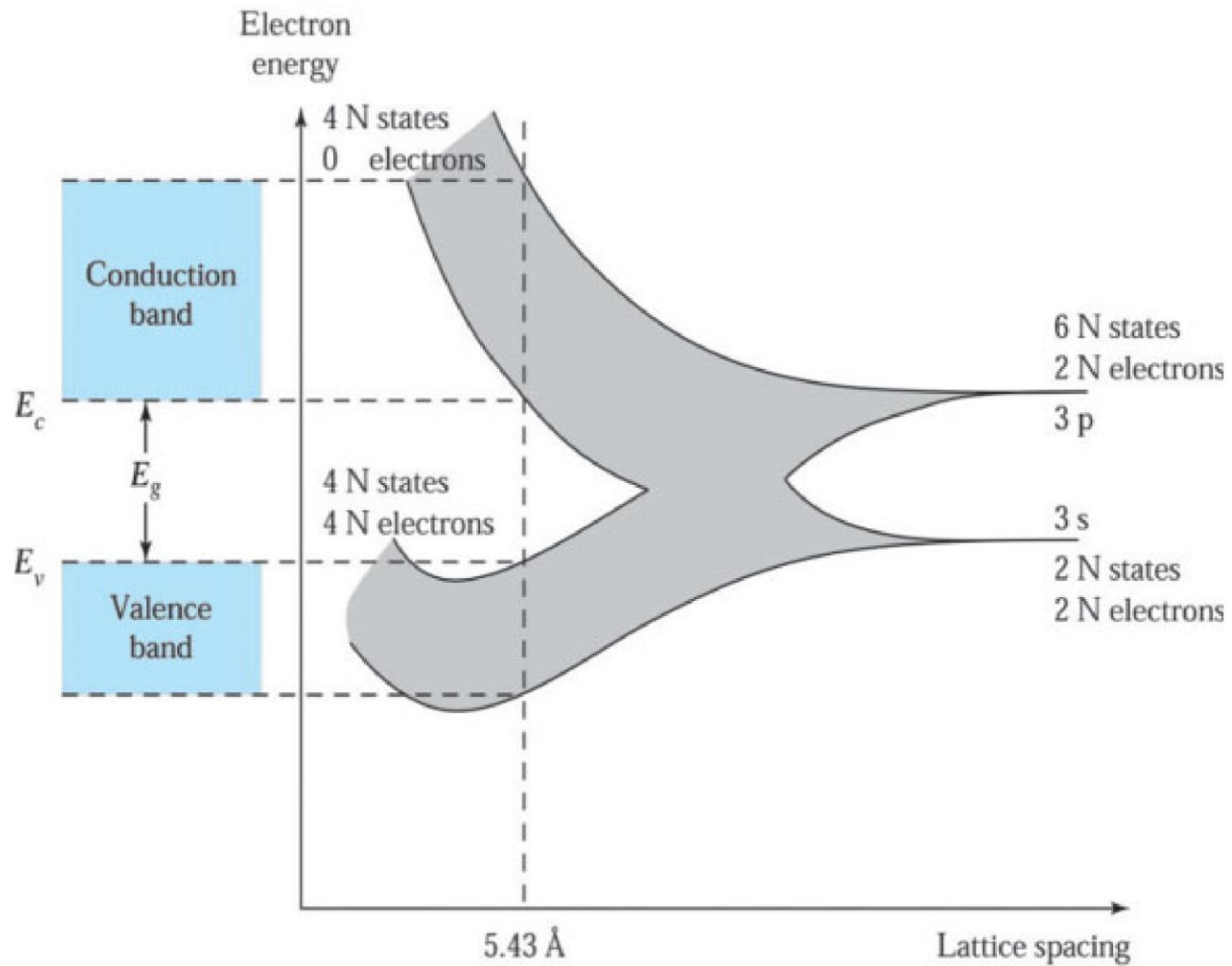


Fig. 10 Schematic representation of an isolated silicon atom.

- The 3s subshell (i.e., for  $n = 3$  and  $\ell = 0$ ) has two allowed quantum states per atom. This subshell will contain two valence electrons at  $T = 0$  K.
- The 3p subshell (i.e.,  $n = 3$  and  $\ell = 1$ ) has six allowed quantum states per atom. This subshell will contain the remaining two valence electrons of an individual silicon atom.
- Figure 11 is a schematic diagram of the formation of a silicon crystal from  $N$  isolated silicon atoms.
- As the interatomic distance decreases, the 3s and 3p subshell of the  $N$  silicon atoms will interact and overlap to form bands.



**Fig. 11** Formation of energy bands as a diamond lattice crystal is formed by bringing isolated silicon atoms together.

- As the 3s and 3p bands grow, they merge (ترکیب شدن) into a single band containing  $8N$  states.
- At the equilibrium interatomic distance determined by the condition of minimum total energy, the bands will again split, with  $4N$  states in the lower band and  $4N$  states in the upper band.
- At a temperature of absolute zero, electrons occupy the lowest energy states, 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 bottom of the conduction band is called  $E_C$  and the top of the valence band is called  $E_V$ .
- The bandgap energy  $E_g$  between the bottom of the conduction band and the top of the valence band ( $E_C - E_V$ ) is the width of the forbidden energy gap, as shown at the far left of Fig. 11.
- Physically,  $E_g$  is the energy required to break a bond in the semiconductor to free an electron to the conduction band and leave a hole in the valence band.

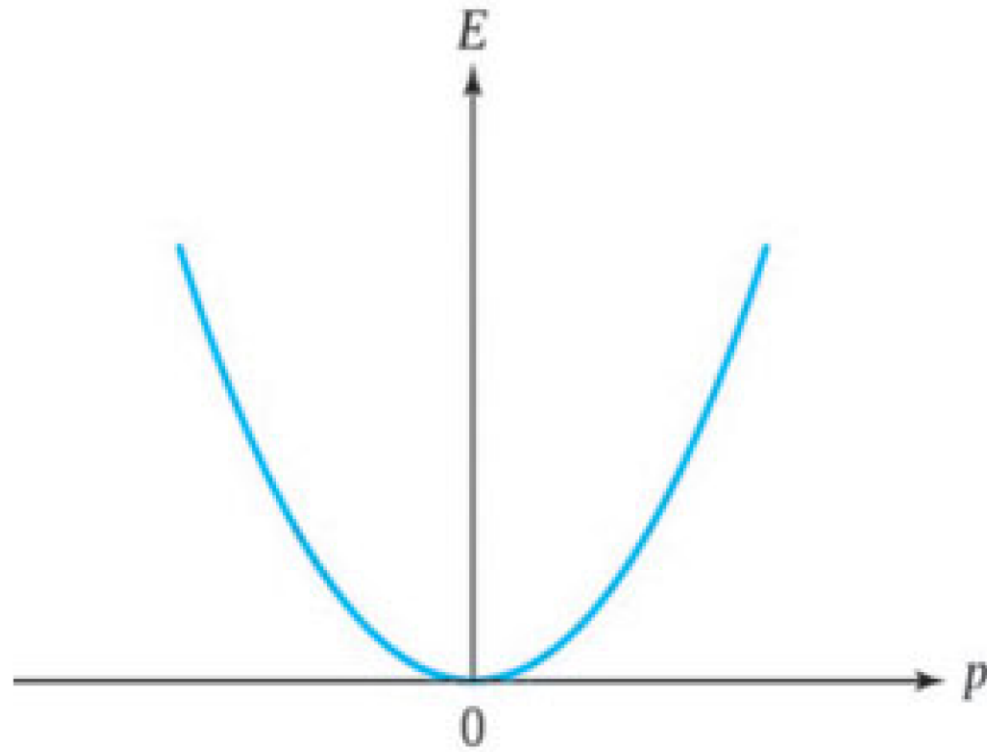
## 1.4.2 The Energy-Momentum Diagram

- The energy  $E$  of a free electron is given by

$$E = \frac{p^2}{2m_0}, \quad (3)$$

where  $p$  is the momentum and  $m_0$  is the free-electron mass.

- If we plot  $E$  vs.  $p$ , we obtain a parabola as shown in Fig. 12.
- In a semiconductor crystal, an electron in the conduction band is similar to a free electron in being relatively free to move about in the crystal. However, because of the periodic potential of the nuclei, Eq. 3 can no longer be valid.



**Fig. 12** The parabolic energy ( $E$ ) vs. momentum ( $p$ ) curve for a free electron.



- However, it turns out that we can still use Eq. 3 if we replace the free-electron mass in Eq. 3 by an effective mass  $m_n$  (the subscript n refers to the negative charge on an electron), that is,

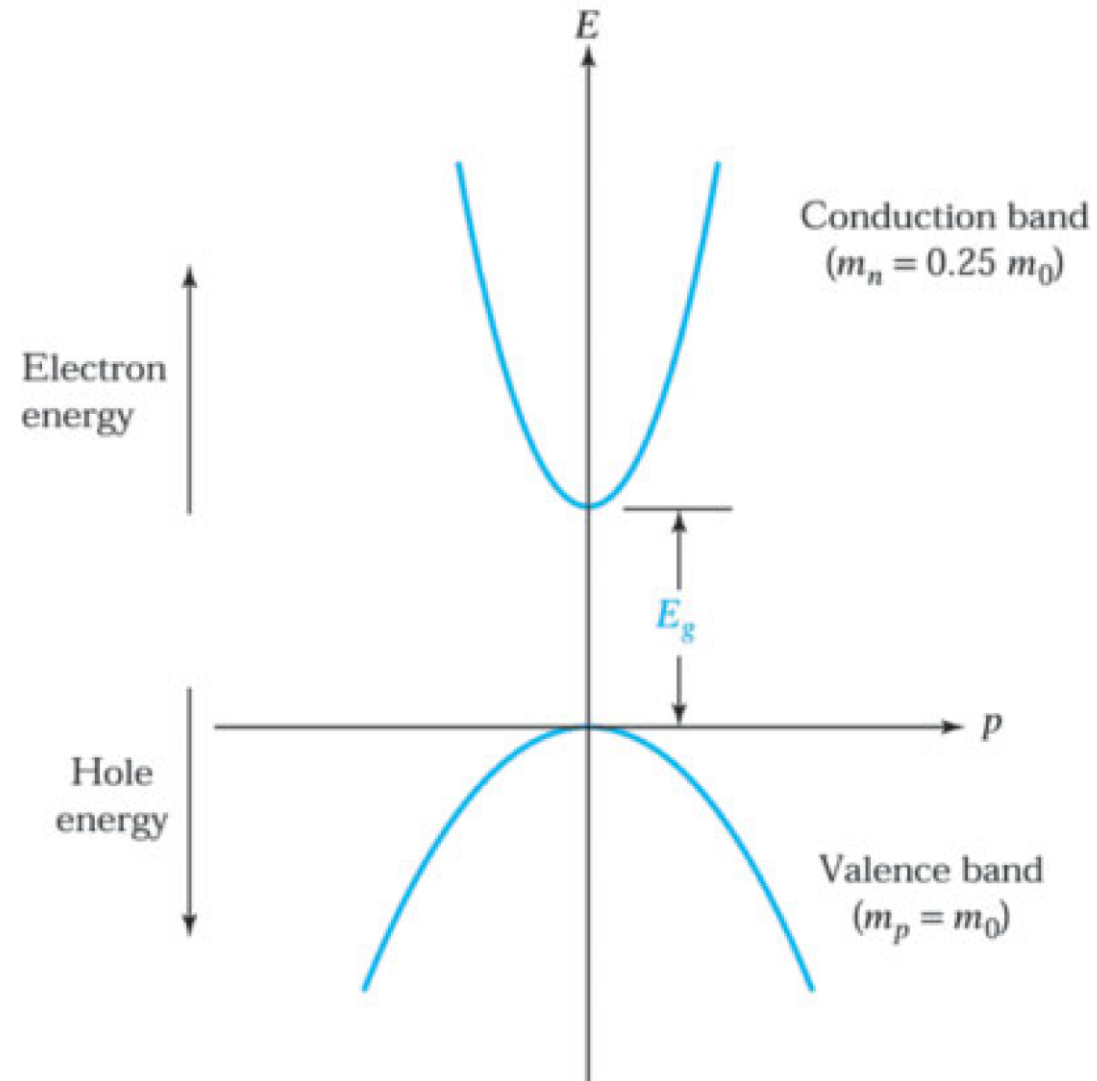
$$E = \frac{p^2}{2m_n}. \quad (4)$$

- The electron effective mass depends on the properties of the semiconductor.
- If we have an energy-momentum relationship described by Eq. 4, we can obtain the effective mass from the second derivative of E with respect to p:

$$m_n \equiv \left( \frac{d^2 E}{dp^2} \right)^{-1}. \quad (5)$$

- Therefore, the narrower the parabola, corresponding to a larger second derivative, the smaller the effective mass. ↓
- A similar expression can be written for holes (with effective mass  $m_p$  where the subscript p refers to the positive charge on a hole).
- The effective-mass concept is very useful because it enables us to treat electrons and holes essentially as classical charged particles.

- Figure 13 shows a simplified energy-momentum relationship of a special semiconductor with an electron effective mass of  $m_n = 0.25m_0$  in the conduction band (the upper parabola) and a hole effective mass of  $m_p = m_0$  in the valence band (the lower parabola).
- Note that the electron energy is measured upward (بطرف بالا) and the hole energy is measured downward.
- The spacing at  $p = 0$  between these two parabolas is the bandgap  $E_g$ , shown previously in Fig. 11.



**Fig. 13** A schematic energy-momentum diagram for a special semiconductor with  $m_n = 0.25 m_0$  and  $m_p = m_0$ .