

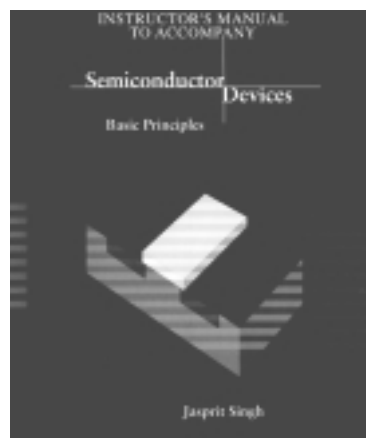
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# Chapter

# 2

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## ELECTRONS IN SEMICONDUCTORS



In this chapter we present figures discussing the behavior of electrons in crystalline solids.

ELECTRONS IN PERIODIC STRUCTURES:  
ELECTRONIC BANDSTRUCTURE ( $E$  vs.  $k$  relation)

To examine electrons inside a solid we need to use quantum mechanics, i.e., the Schrödinger equation

$$\left[ \frac{-\hbar^2}{2m_o} \nabla^2 + V(\mathbf{r}) \right] \psi(\mathbf{r}) = E \psi(\mathbf{r})$$

$\psi(\mathbf{r})$ : electronic state or wavefunction.

$E$  : electronic allowed energy or eigenvalue.

$V(\mathbf{r})$ : background potential which is periodic in crystals.

In general the problem is extremely complex to solve:

There are  $\sim 10^{23}$  atoms  $\text{cm}^{-3}$ !

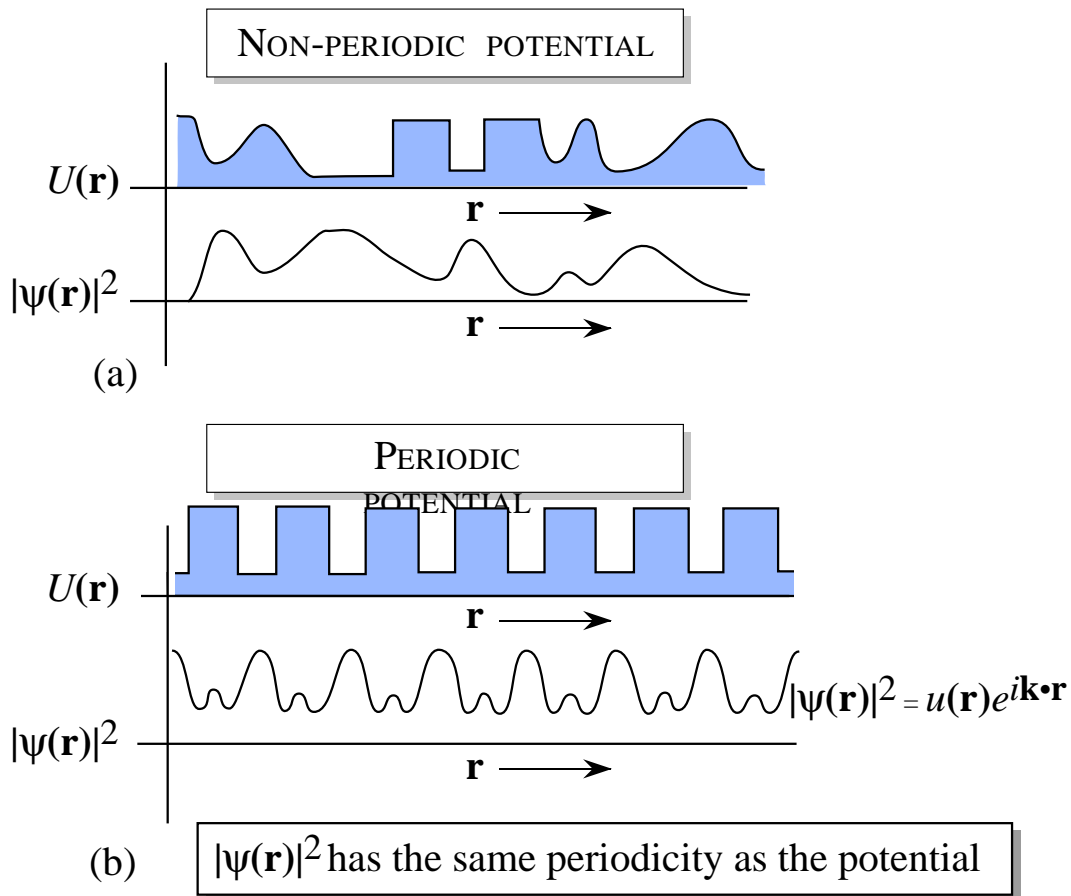
The problem becomes tractable because there is periodicity in the system. The entire crystal is produced by a repetition of a few atoms. This allows us to rewrite the problem in terms of just a unit cell problem.

## BLOCH THEOREM:

The general form of an electronic state (wavefunction) in a periodic structure is:

$$\psi_k(\mathbf{r}) = u_k(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}$$

$u_k(\mathbf{r}) = u_k(\mathbf{r}+R)$ :  $u_k(\mathbf{r})$  has the same periodicity as the crystal.



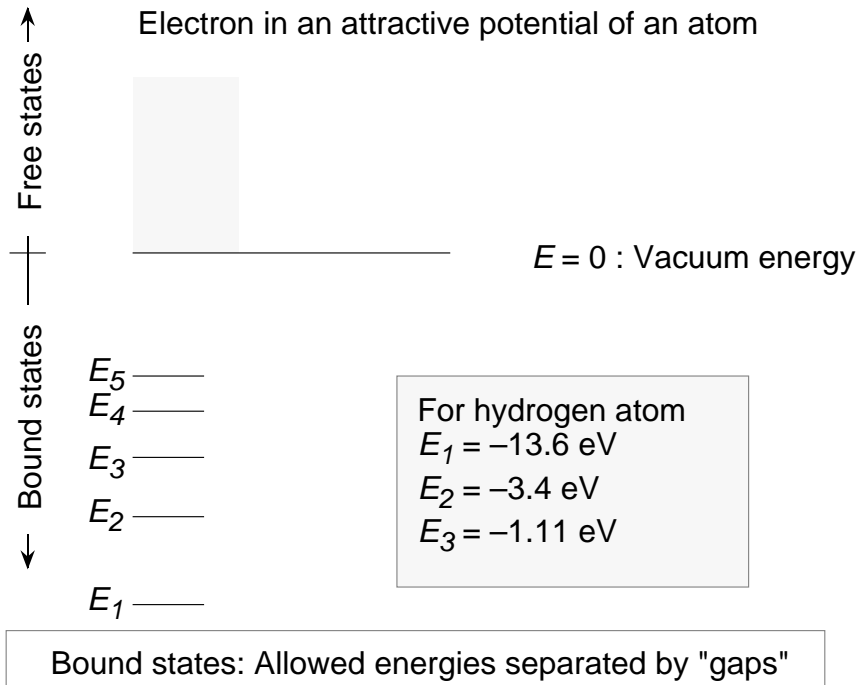
Note that the wavefunction is not periodic.

$k$  is called the crystal momentum.

$u_k(\mathbf{r})$  is called the cell periodic part of the wavefunction.

## ELECTRONS IN AN ATOM

Before examining electrons in a solid, let us examine electronic states in an atom. Let us examine the hydrogen atom.



Allowed energy levels:

$$E_n = \frac{-me^4}{2(4\pi\epsilon_0)^2\hbar^2n^2} = \frac{13.6}{n^2} \text{ eV}$$

Wavefunctions:

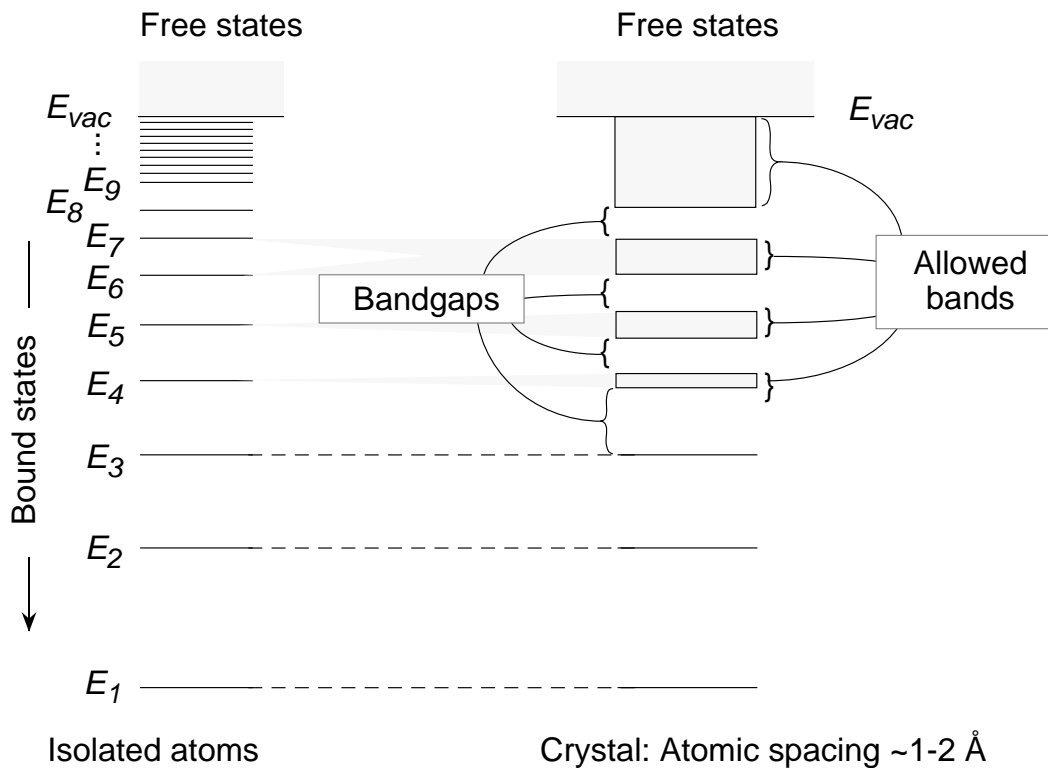
$\psi_{nlm}$ :  $n$ : principle quantum number.

$\ell$ : orbital quantum number; angular momentum of the electron =  $\ell\hbar$ .

$m$ : magnetic quantum number; projection of the angular momentum;  $m$  lies between  $-\ell$  and  $+\ell$ .

## FROM ATOMIC LEVELS TO ENERGY BANDS

As atoms are brought closer and closer to each other to form a crystal, the discrete atomic levels start to broaden to form bands of allowed energies separated by gaps. The electronic states in the allowed bands are Bloch states, i.e., they are plane wave states ( $\sim e^{i\mathbf{k}\cdot\mathbf{r}}$ ).

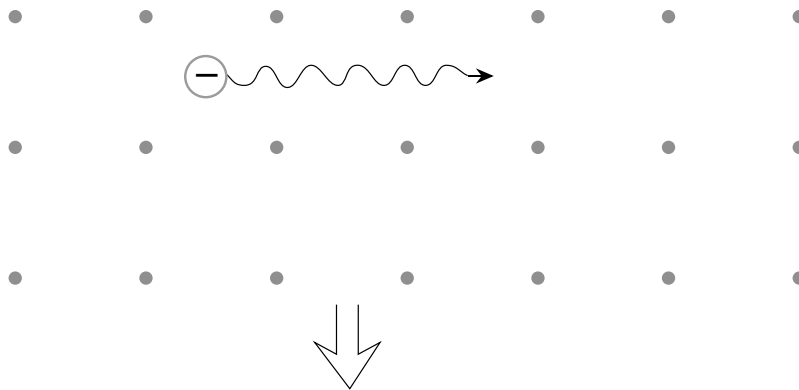


- Low lying core levels are relatively unaffected.
- Higher levels are broadened significantly to form bands.

## ELECTRONS IN A (SOLID) CRYSTAL

Inside a crystal electrons respond to outer forces as if they have an effective momentum  $\hbar k$ . Near the bandedges they respond as if they have an effective mass  $m^*$ .

### ELECTRON WAVE IN A PERIODIC CRYSTAL



Energy solutions of Schrödinger equation:

Series of allowed bands and series of bandgaps.

Properties of the bandgap:

In the perfect crystal, electrons are forbidden from occupying energies in the bandgap.

Properties of an allowed band:

Electrons behave as if they are in free space with a certain wavevector  $k$ . They respond to the outside world as if they have a new mass called the effective mass.

Response to outside forces:

$$\frac{\hbar dk}{dt} = \text{Force}$$

$$E = \frac{\hbar^2 k^2}{2m^*}$$

## FILLING OF ENERGY BANDS: FERMI DISTRIBUTION

At equilibrium electrons fill up the allowed energy states in a way that the free energy is a minimum

Free energy ( $F$ ) = Internal energy ( $U$ ) –  $TS$

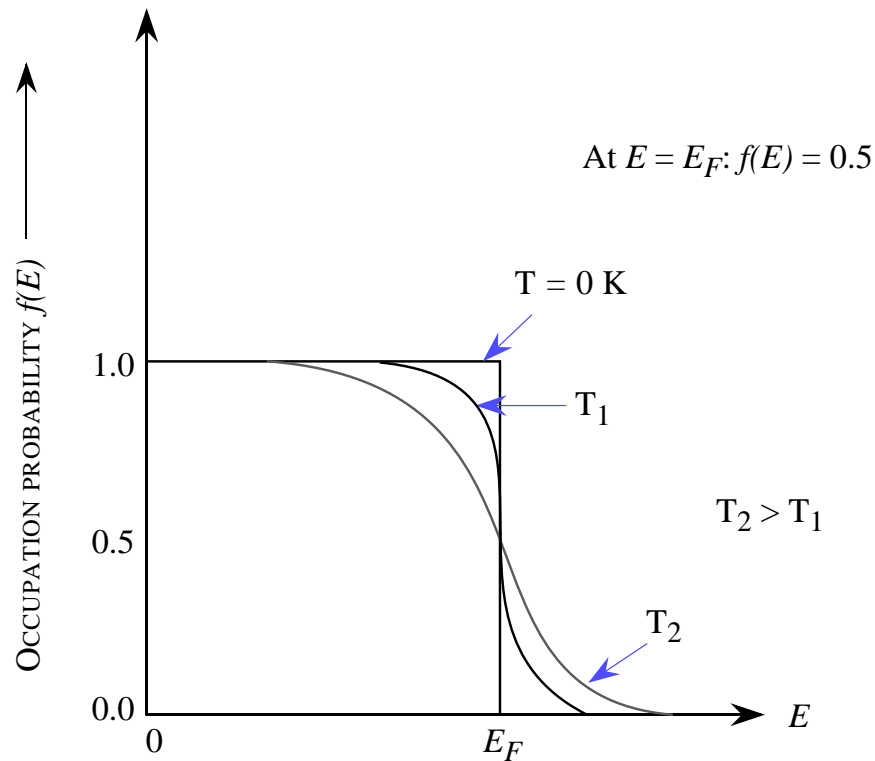
$T$  = Temperature in Kelvin

$S$  = Entropy =  $k\ell nW$

$W$  = Total degeneracy of the electron system.

For electrons (which obey Pauli exclusion principle, i.e., one electron per state) the electron occupation is

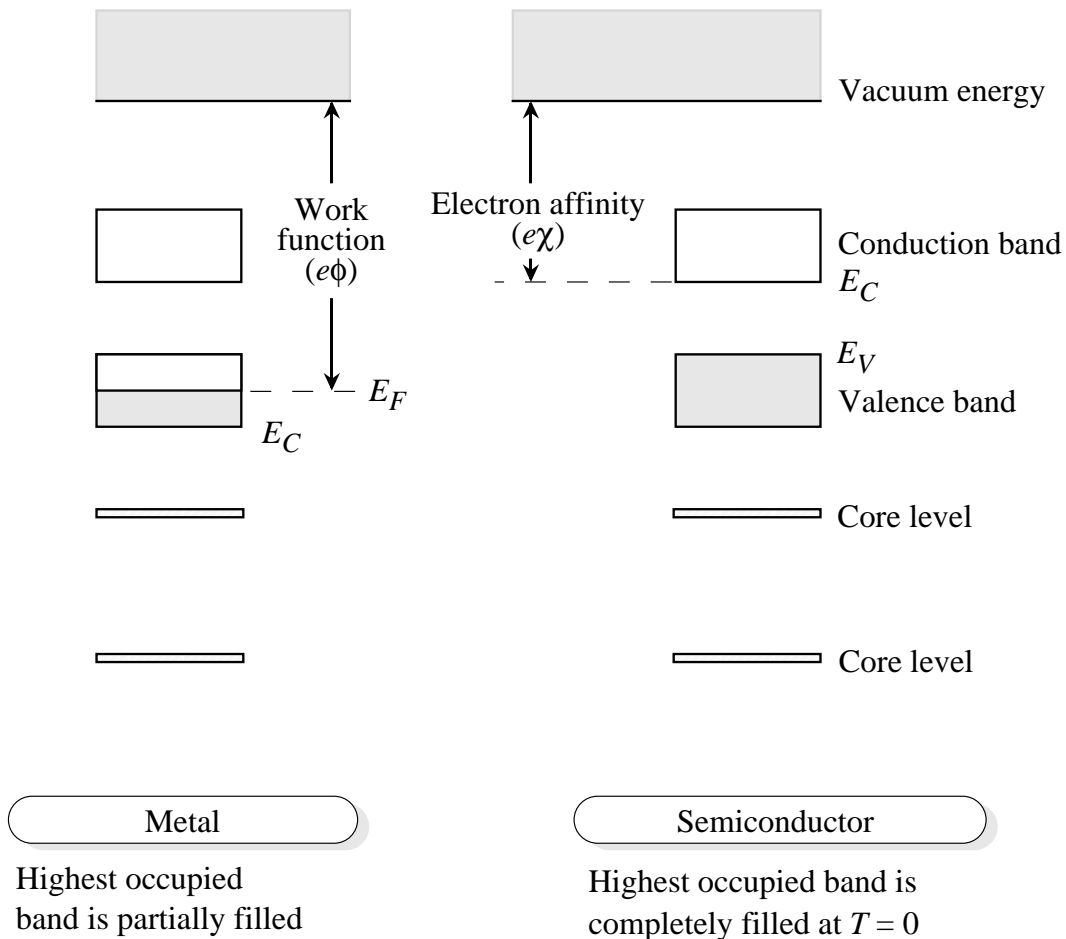
$$f(E) = \frac{1}{1 + \exp \frac{E - E_F}{k_B T}}$$



# METALS, INSULATORS, AND SEMICONDUCTORS

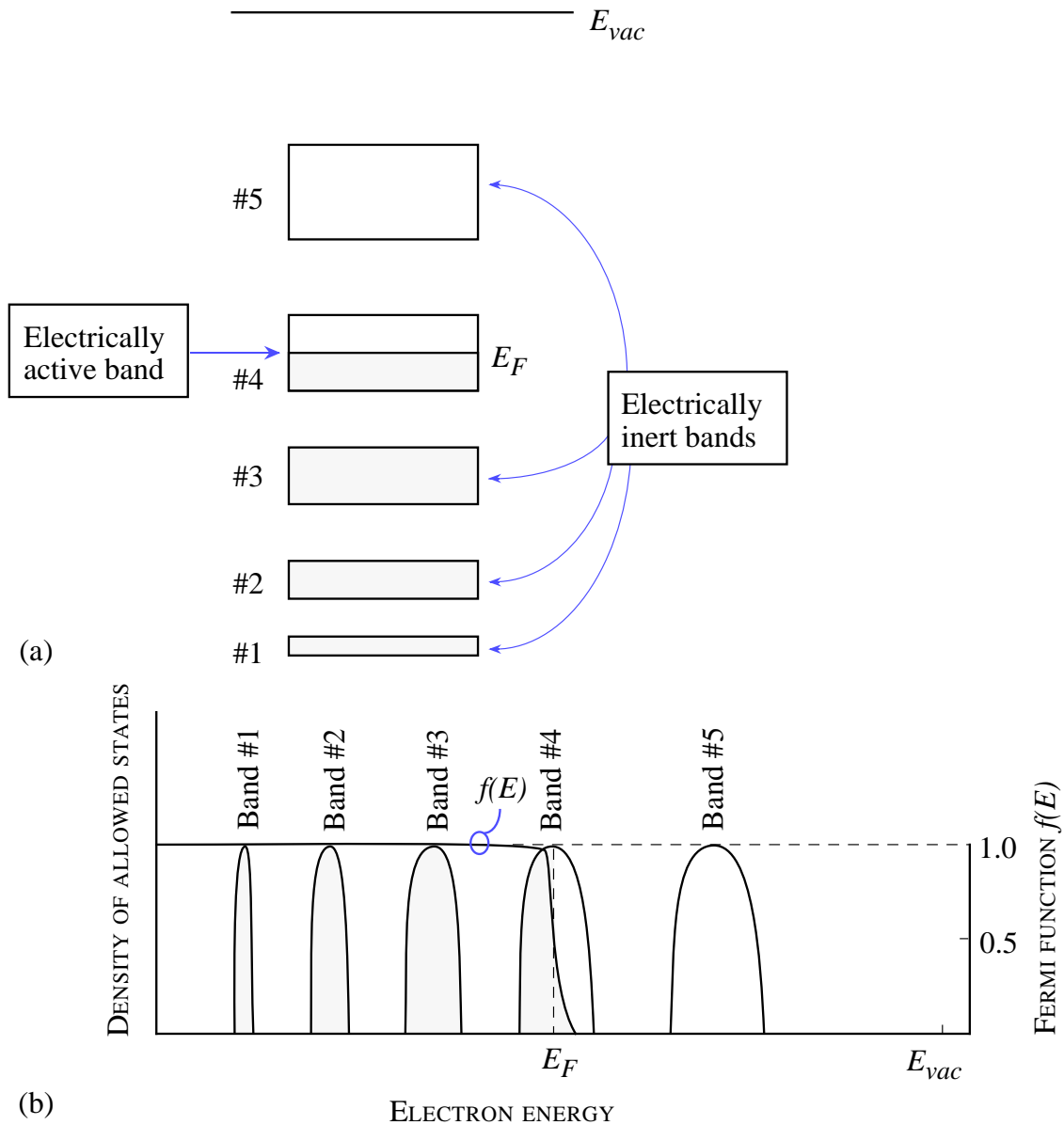
**METALS:** Electron density is such that highest occupied band is partially (say, half) filled.

**INSULATORS/SEMICONDUCTORS:** Highest occupied band is completely filled at low temperature.



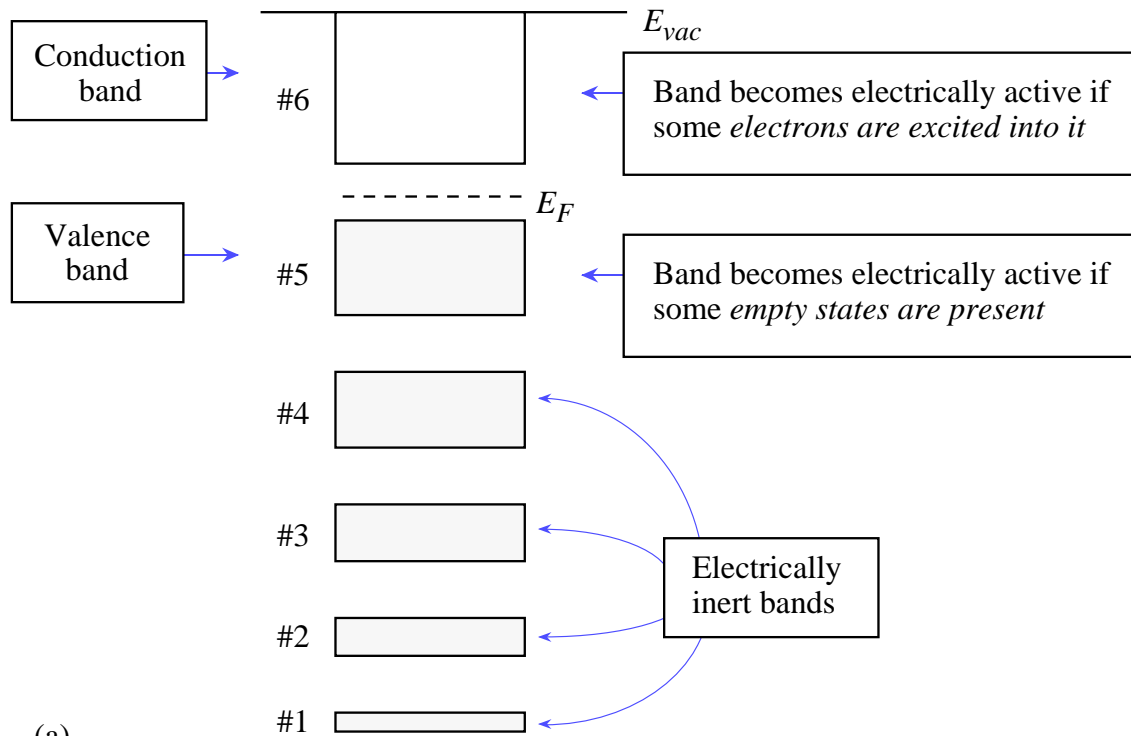
- A completely filled band does not carry any current  $\Leftrightarrow$  Pauli exclusion principle. Electrons need an empty state to move.
- $\Rightarrow$  Insulators and semiconductors have very low conductivity.
- $\Rightarrow$  Metals have a high conductivity.

## EXAMPLE OF ELECTRONS IN A METAL

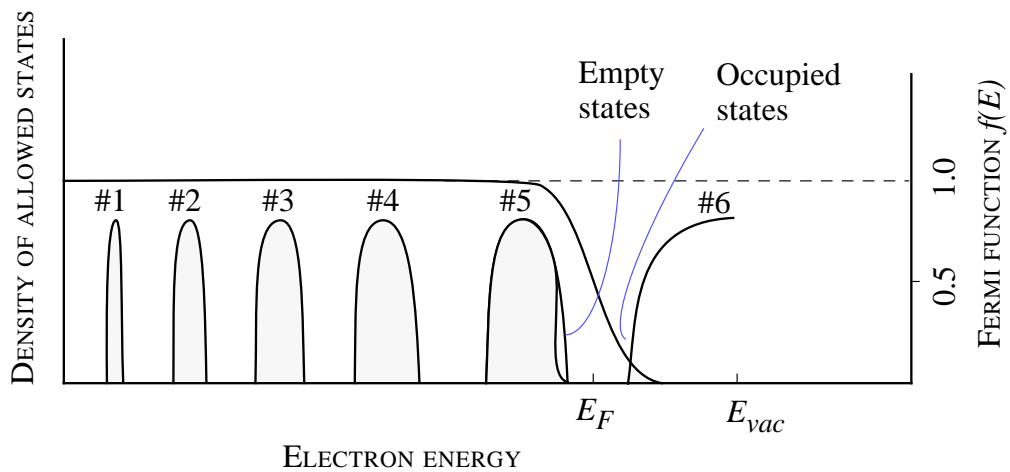


(a) Allowed energy bands and filling of bands by electrons in metals. (b) A schematic of allowed bands and density of states in a metal. In the example shown Band #4 is the conduction band.

## EXAMPLE OF ELECTRONS IN A SEMICONDUCTOR



(a)



(b)

(a) Allowed energy bands and filling of bands in a semiconductor. (b) Density of allowed states in a semiconductor. Here, Band #5 is the valence band and Band #6 is the conduction band.