

Lecture 3

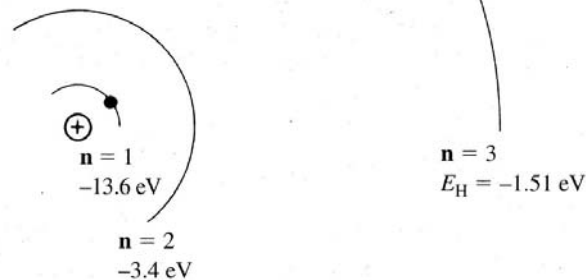
Bonding Model and Dopants

Reading:

(Cont'd) Pierret 1.1, 1.2, 1.4, 2.1-2.6

Comparison of the Hydrogen Atom and Silicon Atom

Hydrogen



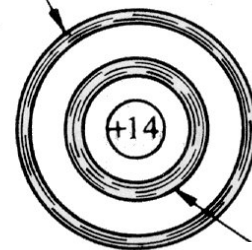
$$Energy_{Hydrogen\ electron} = -\frac{m_o q^4}{2(4\pi \epsilon_o \hbar n)^2} = -\frac{13.6\ eV}{n^2}$$

where m_o = electron mass, \hbar = planks constant / $2\pi = h / 2\pi$
 q = electron charge, and $n = 1, 2, 3, \dots$

Figure 2.1 The hydrogen atom—idealized representation showing the first three allowed electron orbits and the associated energy quantization.

n=2: Complete Shell
 2 “2s electrons”
 6 “2p electrons”
 8 Electrons

Silicon



n=1: Complete Shell
 2 “s electrons”
 n=3:
 2 “3s electrons”
 Only 2 of 6 “3p electrons”

4 empty states

4 Valence Shell Electrons

Six allowed levels at same energy
 Two allowed levels at same energy

Figure 2.2 Schematic representation of an isolated Si atom.

Pauli Exclusion Principle

Only 2 electrons, of spin $\pm 1/2$, can occupy the same energy state at the same point in space.

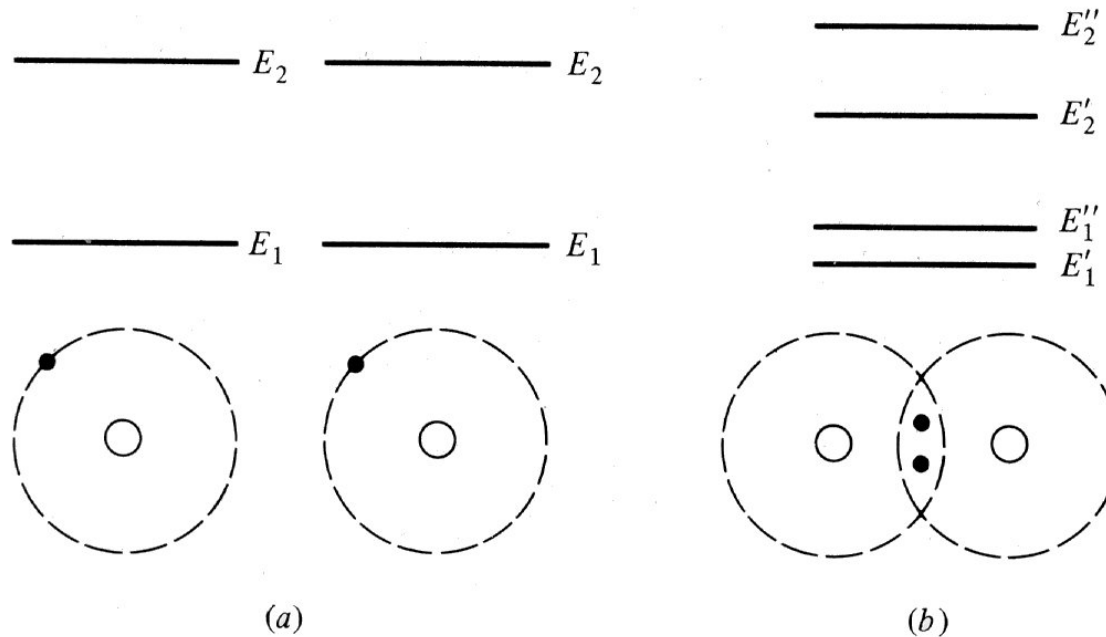
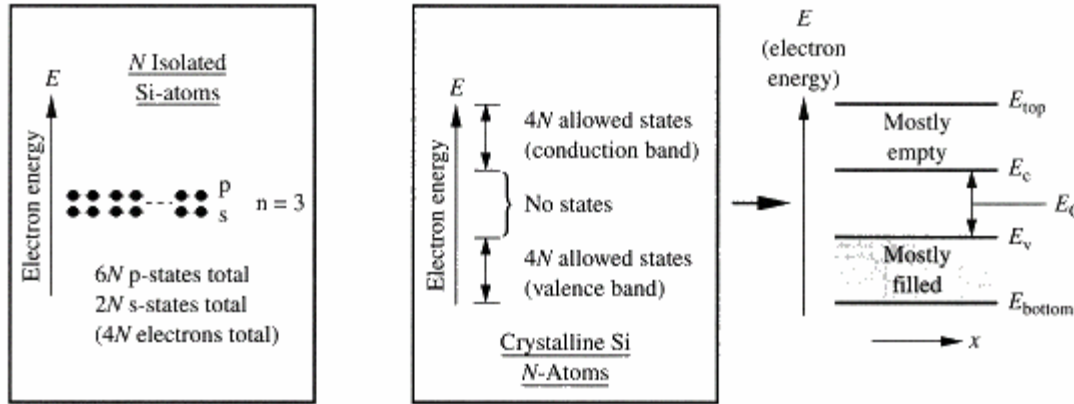


FIGURE 1-9

Two hydrogen atoms: (a) noninteracting and (b) interacting. Splitting of energy levels is illustrated for (b).

Banding of Discrete states and the Simplified Model



T=0K

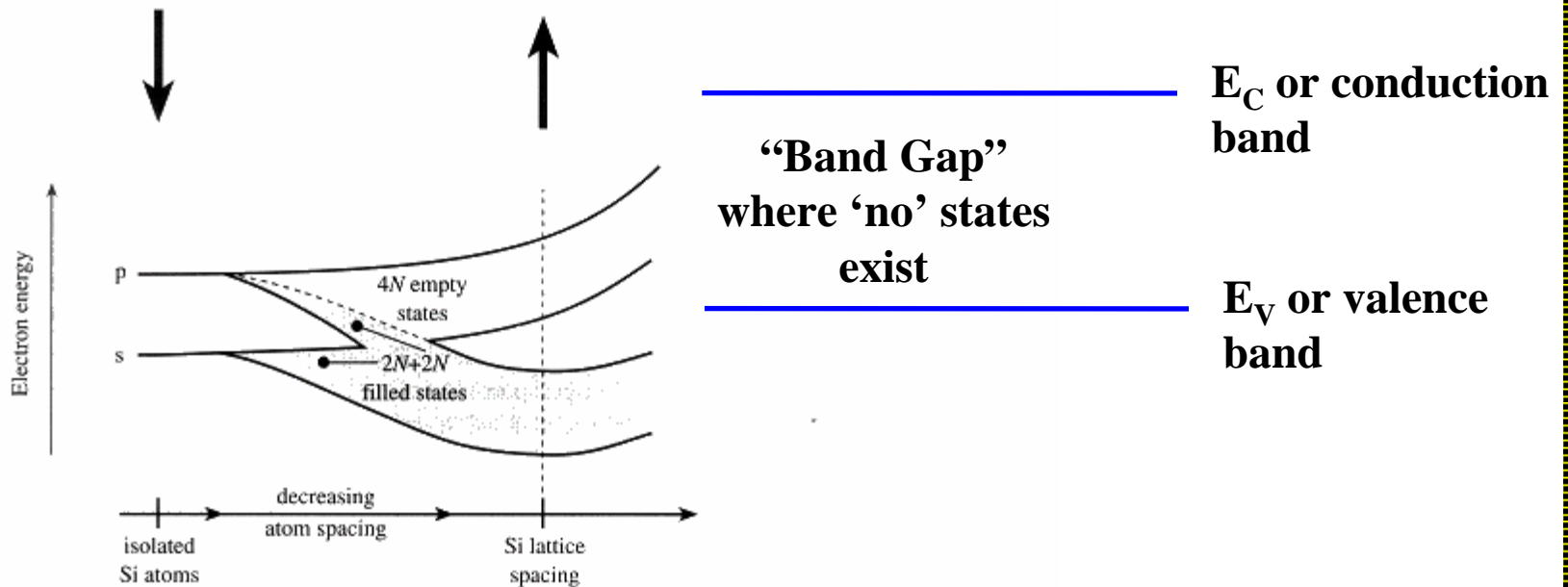
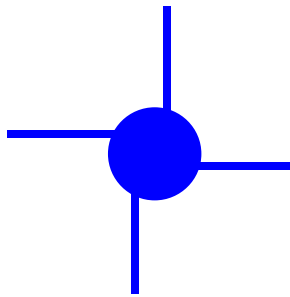
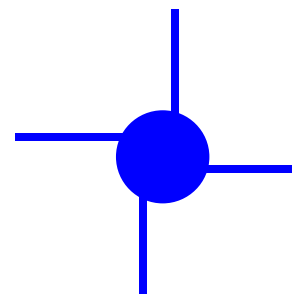
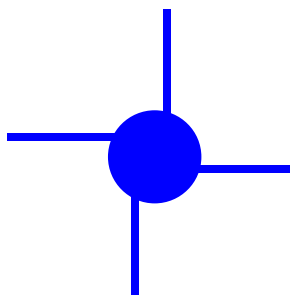
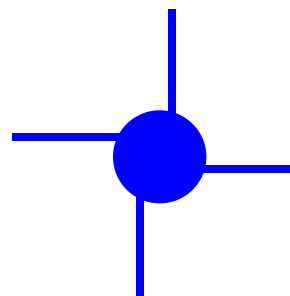
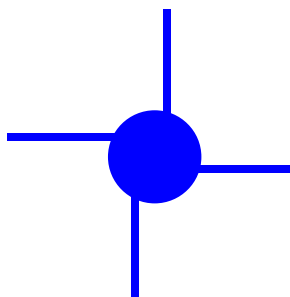


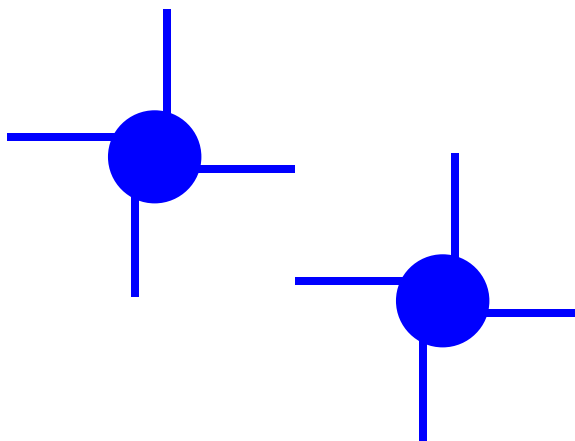
Figure 2.5 Conceptual development of the energy band model starting with N isolated Si atoms on the top left and concluding with a “dressed-up” version of the energy band model on the top right.

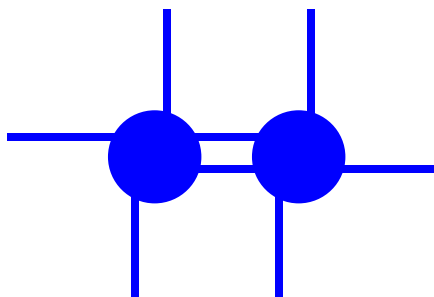


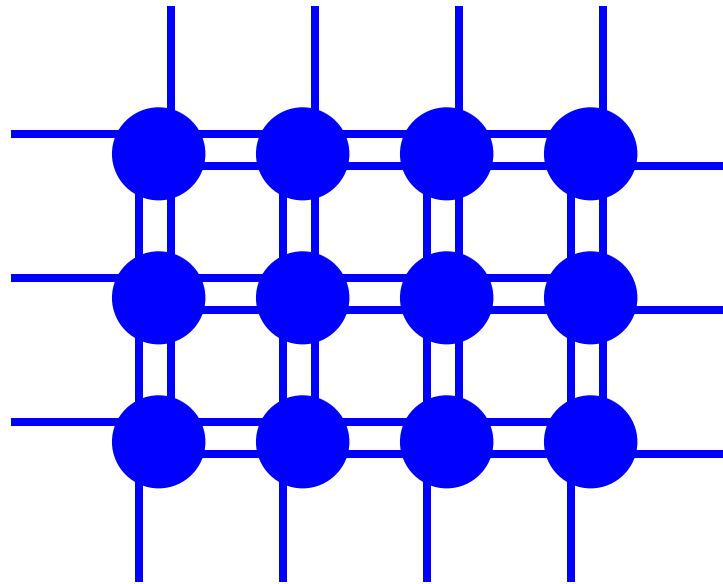
**4 electrons available for sharing
(covalent bonding) in outer shell
of atoms**

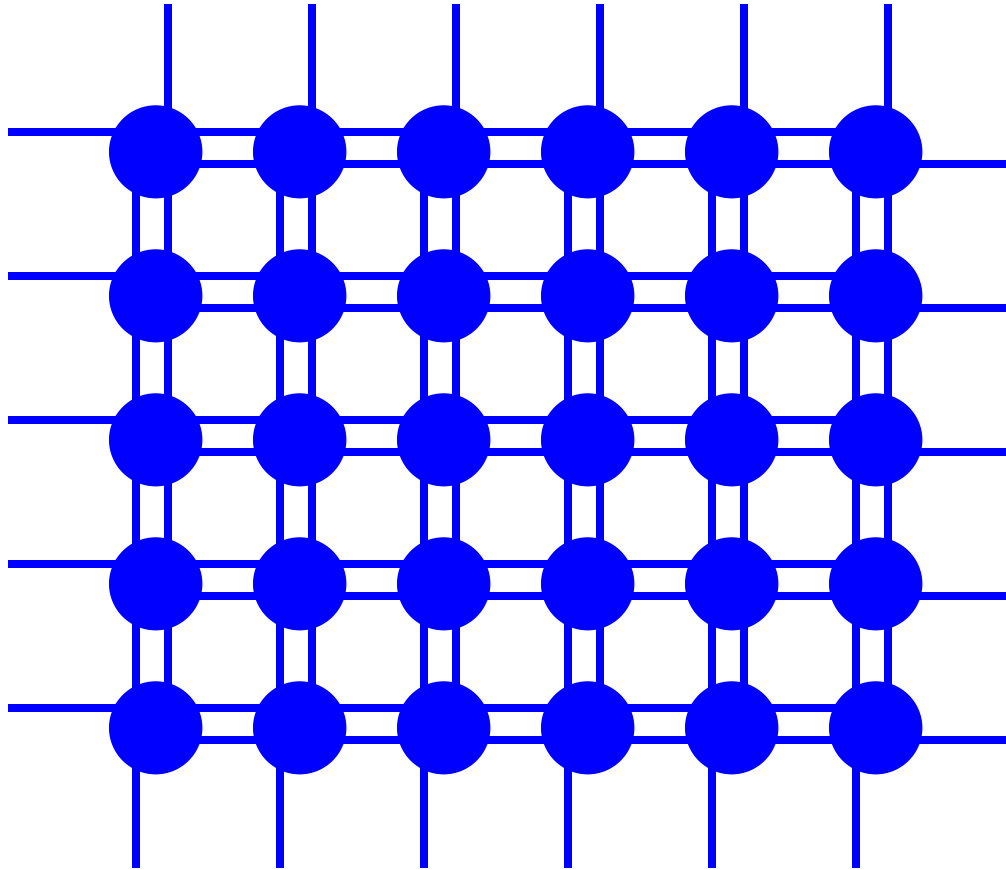


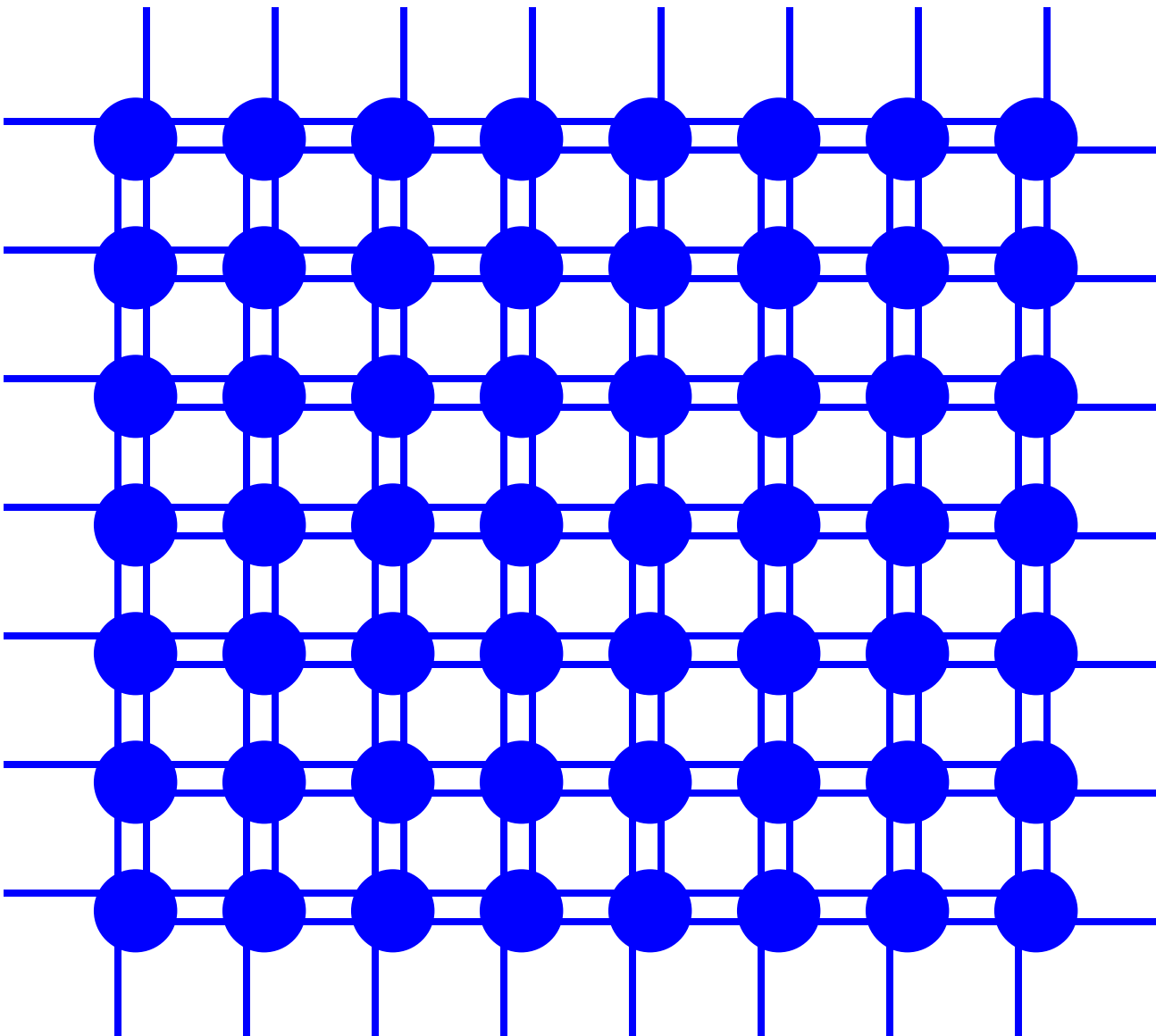






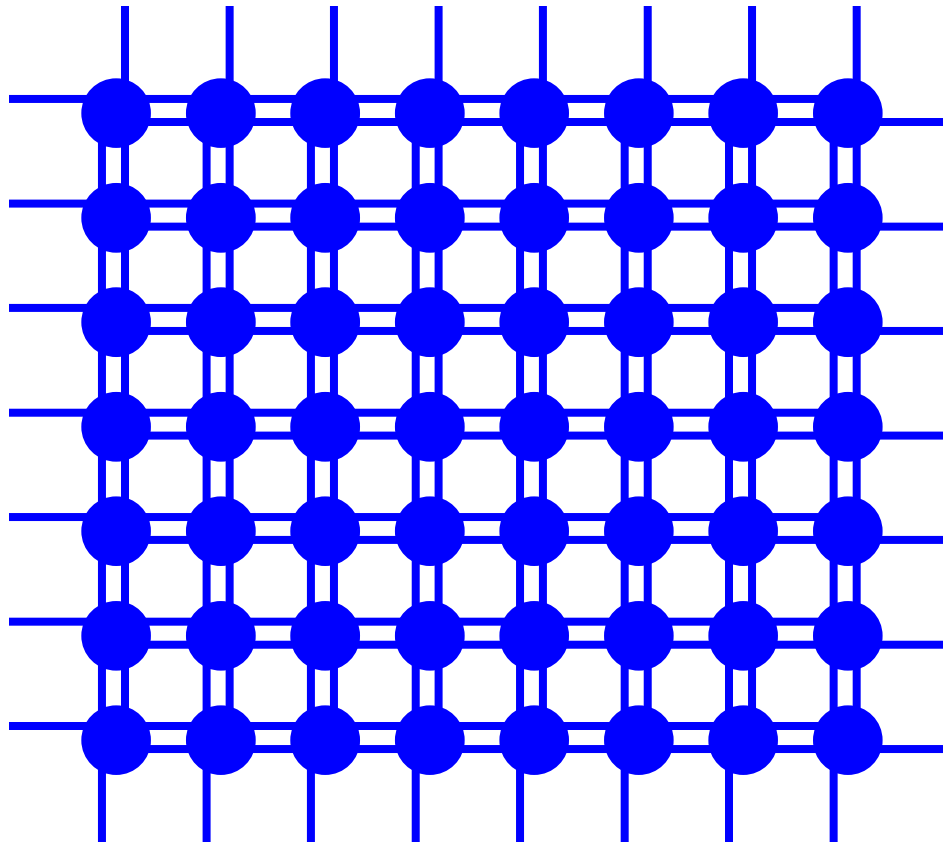






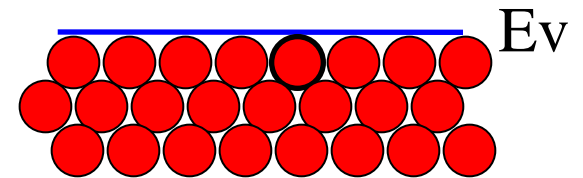
Band Occupation at Low Temperature (0 Kelvin)

For $(E_{\text{thermal}}=kT)=0$



No electrons in conduction band means no electron conduction is possible

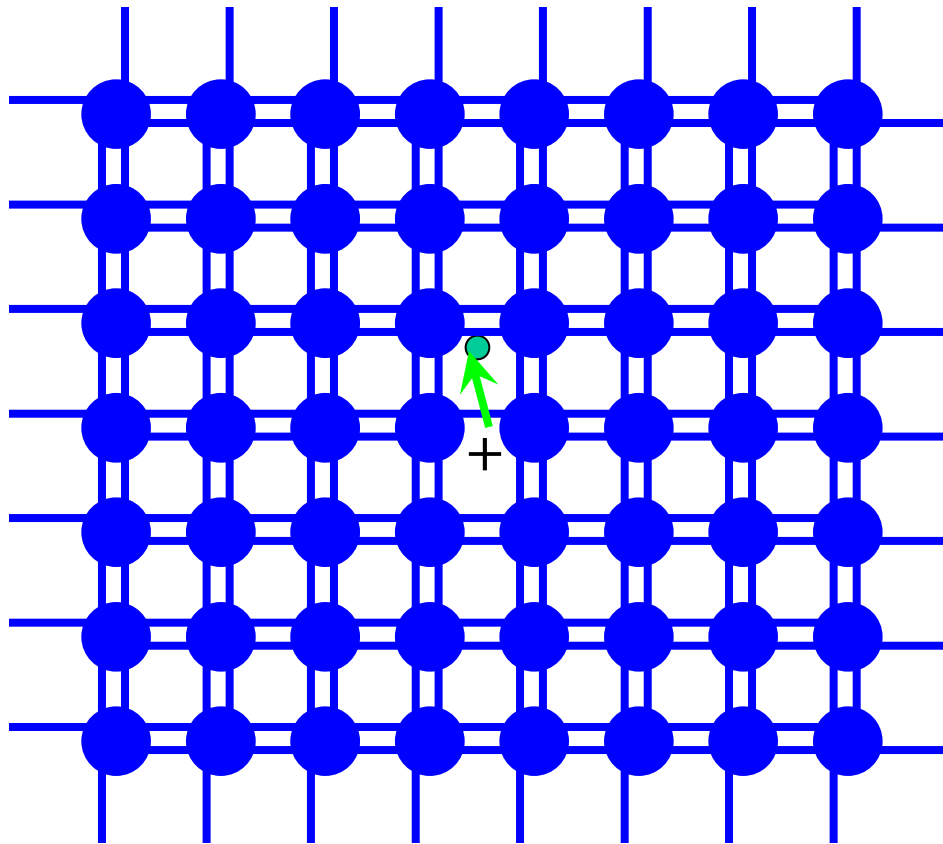
————— E_c



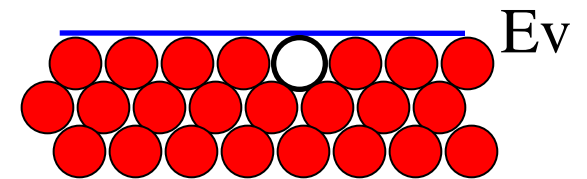
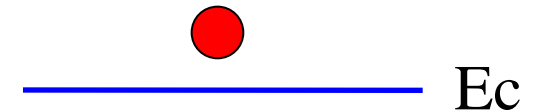
No "Holes" valence band means no "hole" conduction is possible

Band Occupation at Higher Temperature ($T > 0$ Kelvin)

For $(E_{\text{thermal}} = kT) > 0$



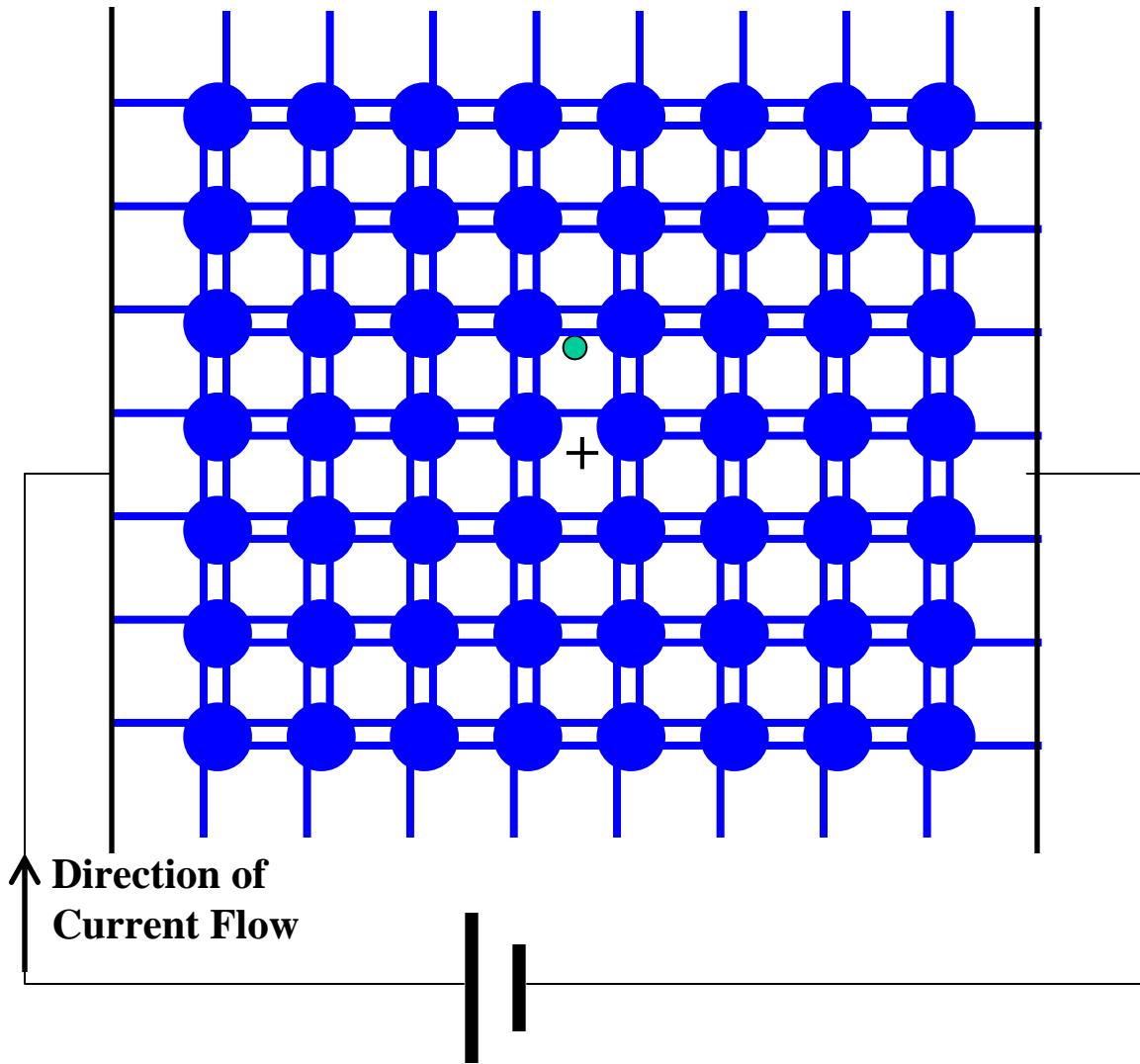
Electron free to move
in conduction band



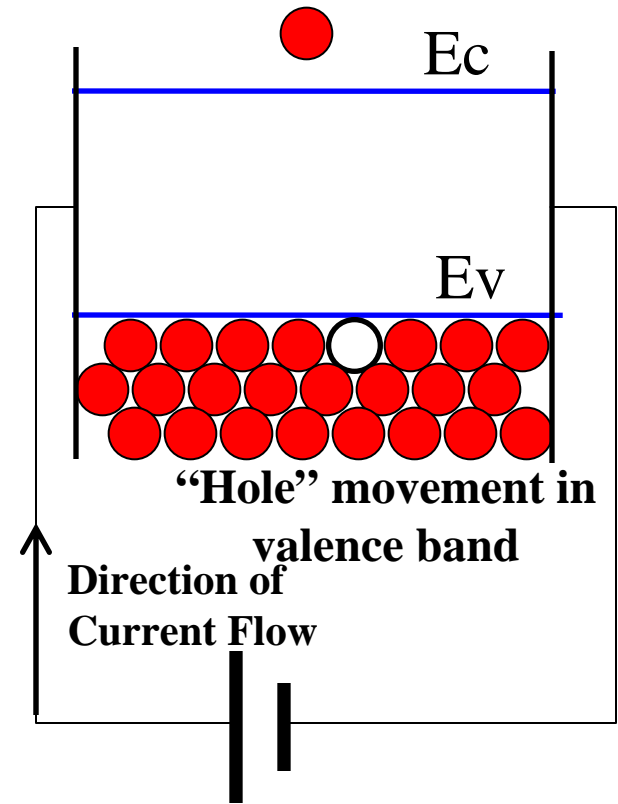
“Hole” free to move in
valence band

Carrier Movement Under Bias

For $(E_{\text{thermal}}=kT) > 0$

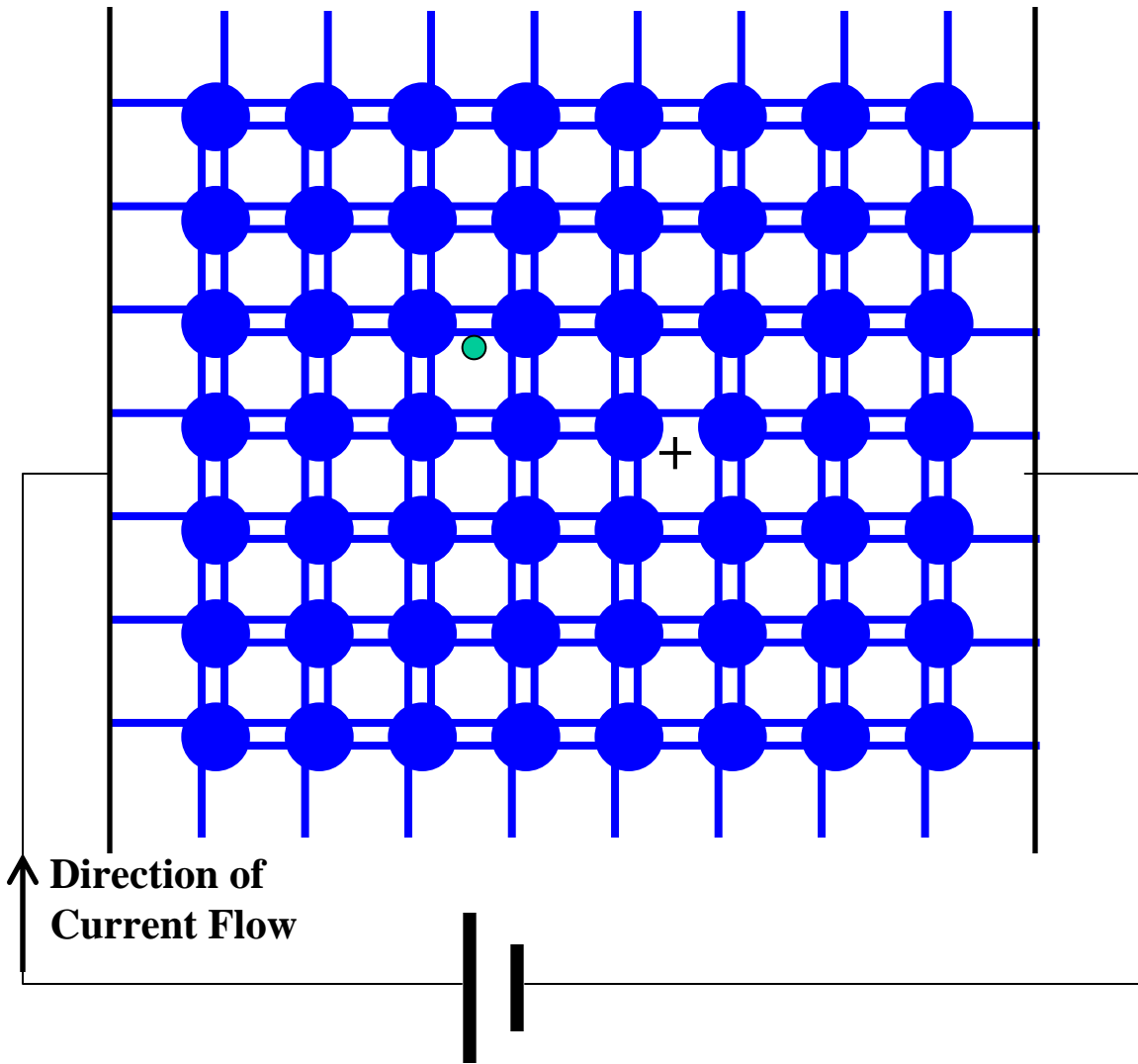


Electron free to move in conduction band

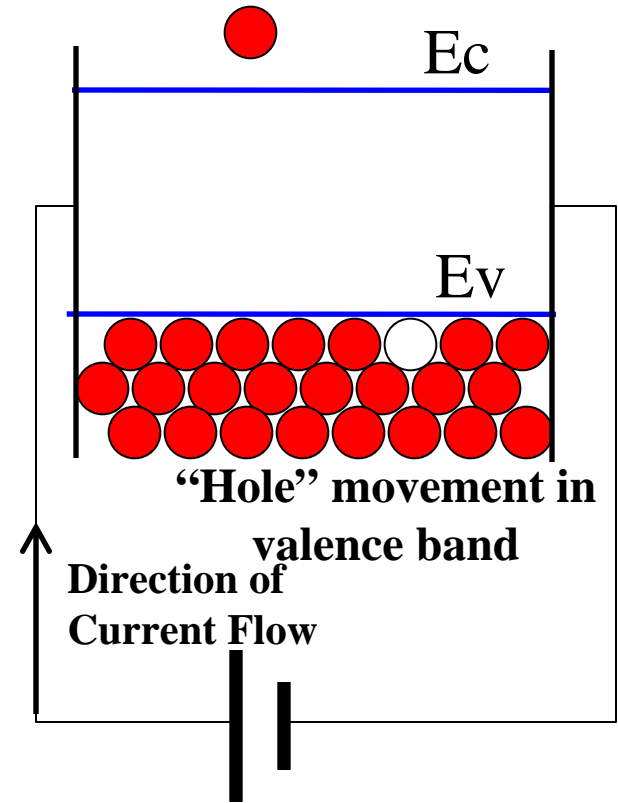


Carrier Movement Under Bias

For $(E_{\text{thermal}}=kT) > 0$

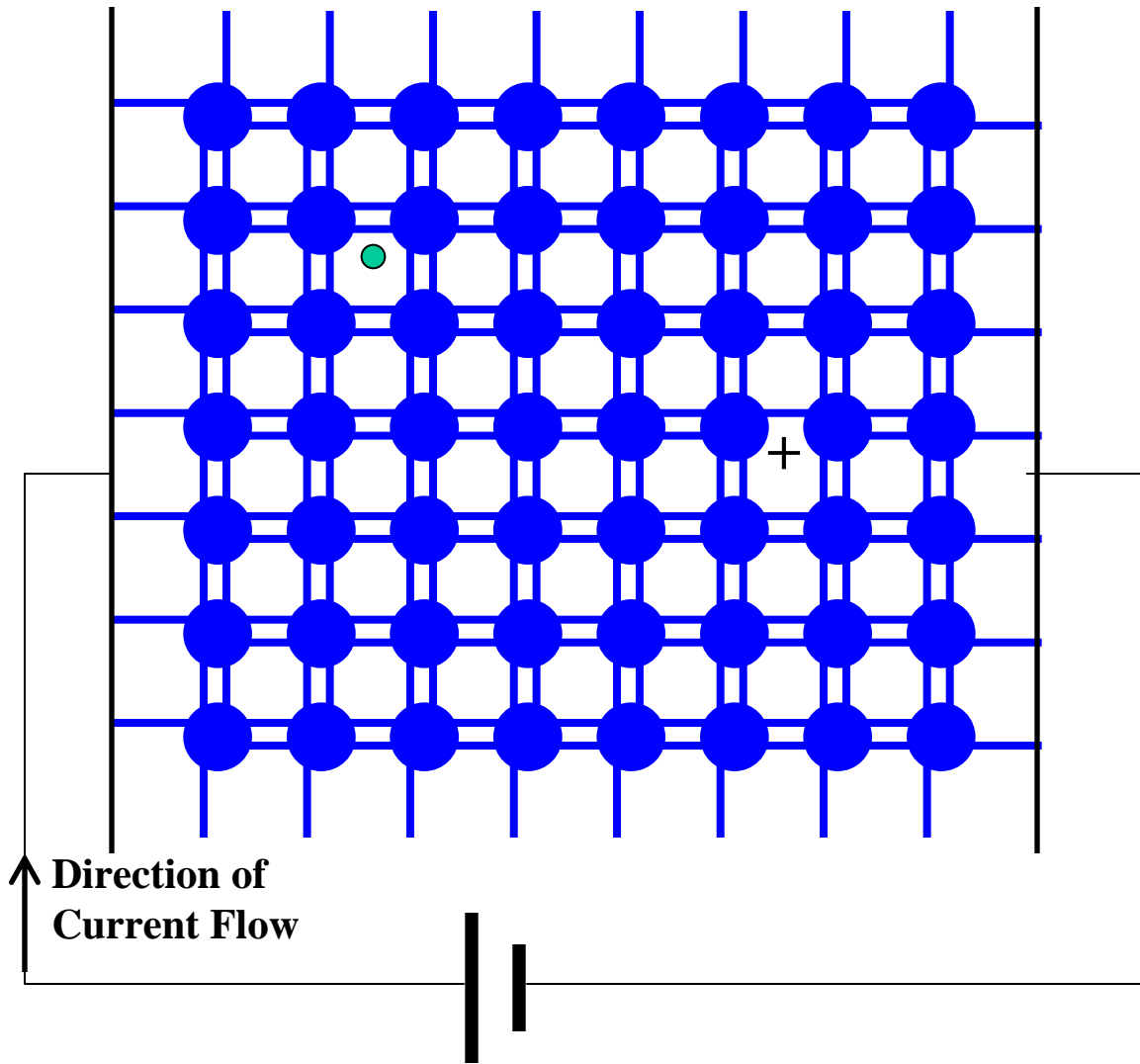


Electron free to move in conduction band

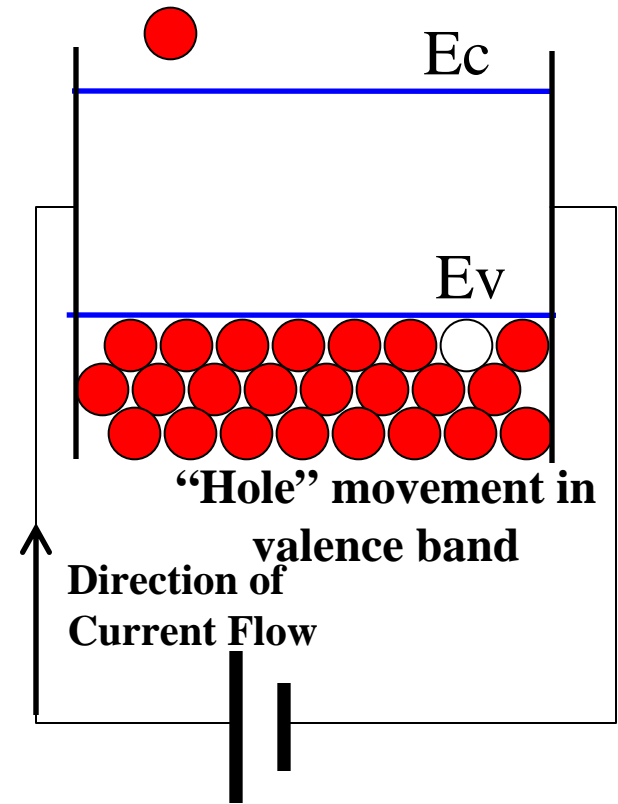


Carrier Movement Under Bias

For $(E_{\text{thermal}}=kT) > 0$



Electron free to move in conduction band



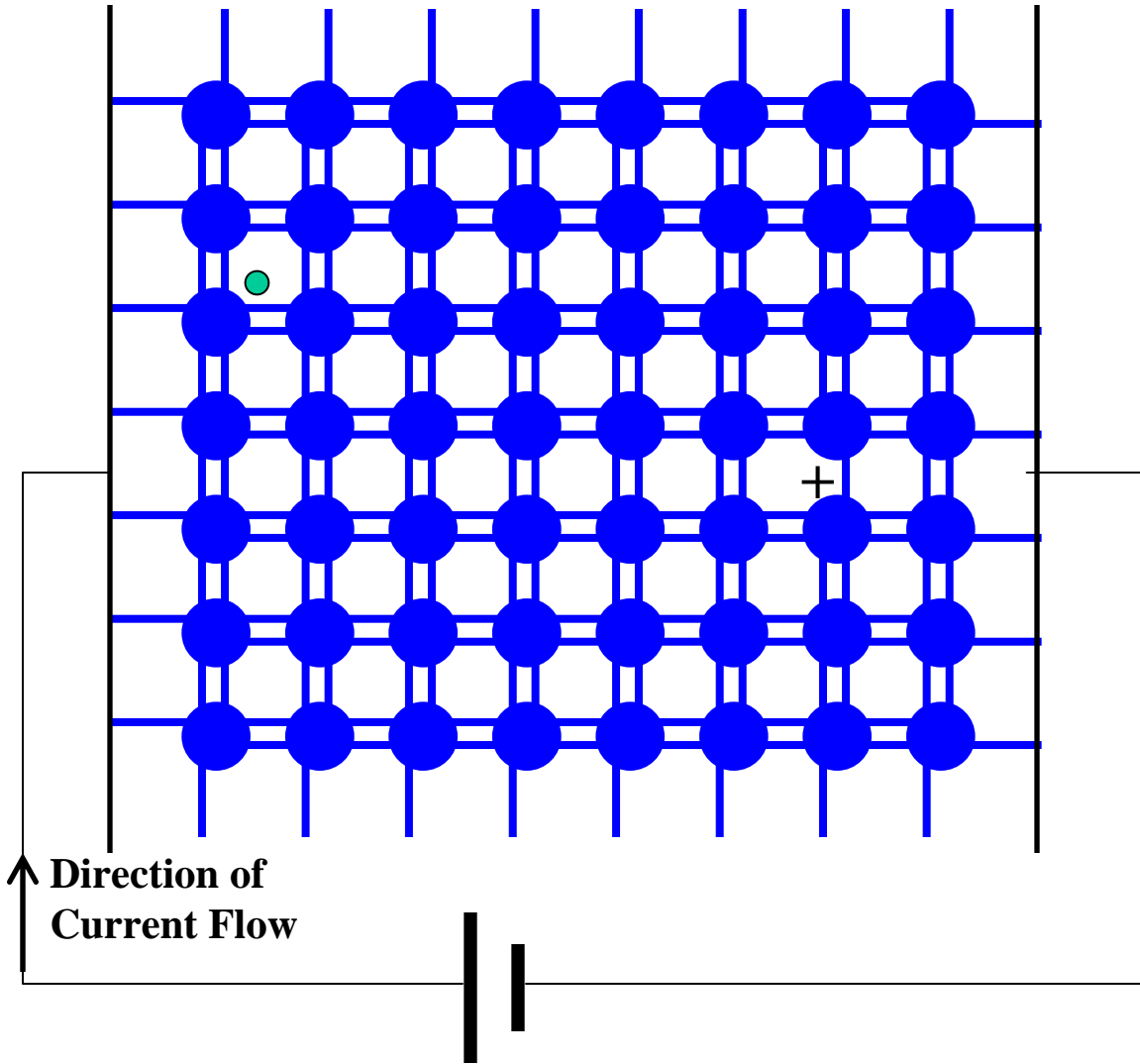
"Hole" movement in valence band

Carrier Movement Under Bias

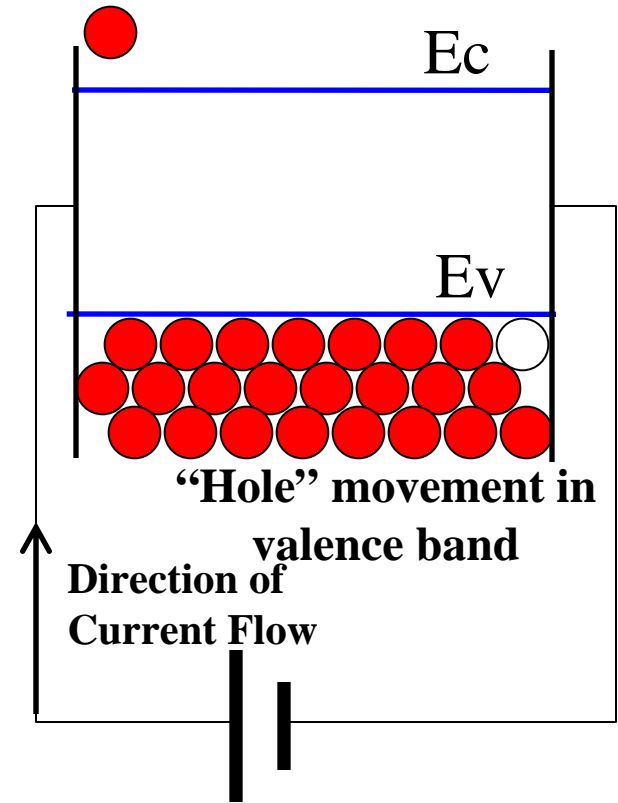


QuickTime Movie

For $(E_{\text{thermal}}=kT) > 0$

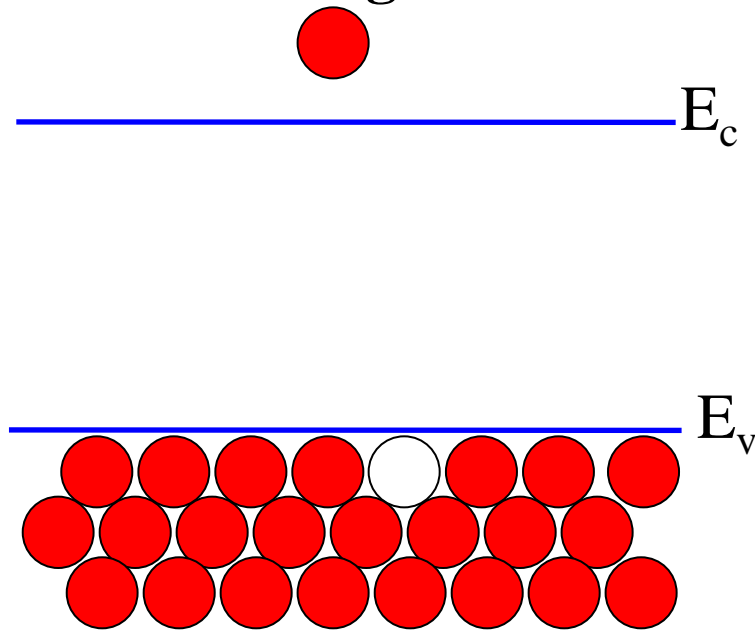


Electron free to move in conduction band



"Hole" movement in valence band

Clarification of confusing issues: “Holes” and Electrons



The valence band may have $\sim 4 \times 10^{22} \text{ cm}^{-3}$ valence electrons “participating in the bonding processes holding the crystal together.

The valence band might only have $\sim 10^6$ to 10^{19} cm^{-3} “holes” in the valence band (missing valence electrons). Thus, it is easier to account for the influence of the holes by counting the holes directly as opposed to counting very small changes in the valence electron concentrations.

Example: If there are 10^{22} cm^{-3} atoms in a crystal with each atom having 4 valence electrons. What is the difference in valence electron concentration for 10^{12} holes versus 10^{13} cm^{-3} holes?

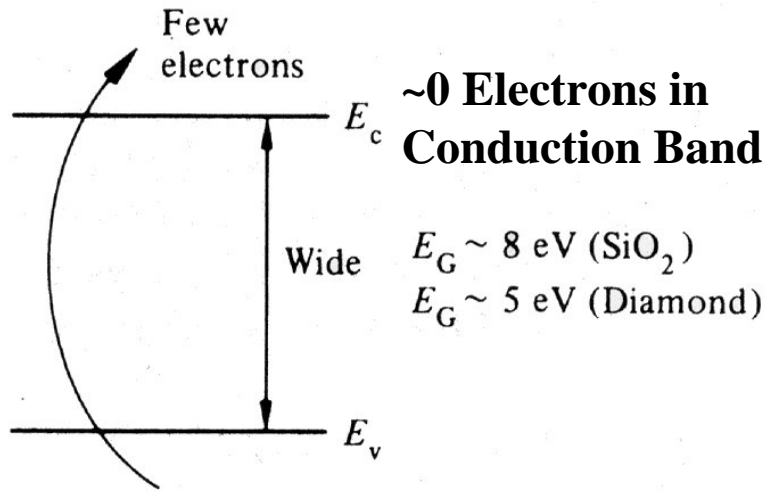
$$\text{Answer: } 4 \times 10^{22} \text{ cm}^{-3} - 10^{12} \text{ cm}^{-3} = 3.9999999999 \times 10^{22} \text{ cm}^{-3} \text{ verses}$$

$$4 \times 10^{22} \text{ cm}^{-3} - 10^{13} \text{ cm}^{-3} = 3.9999999999 \times 10^{22} \text{ cm}^{-3}$$

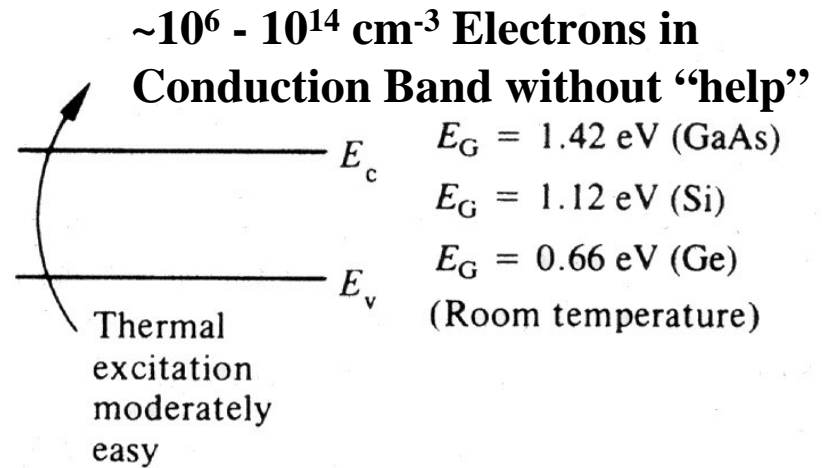
For “accounting reasons” keeping track of holes is easier!

Material Classification based on Size of Bandgap:

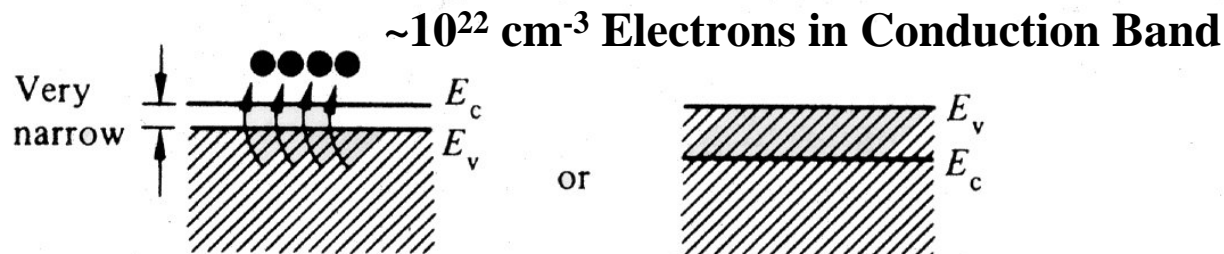
Ease of achieving thermal population of conduction band determines whether a material is an insulator, semiconductor, or metal



(a) Insulator



(b) Semiconductor



(c) Metal

Figure 2.8 Explanation of the distinction between (a) insulators, (b) semiconductors, and (c) metals using the energy band model.

Intrinsic Carrier Concentration

- For each electron promoted to the conduction band, one hole is left in the valence band. Thus, the number of electrons in the conduction band is equal to the number of holes in the valence band unless there is “help” to change the relative populations in each band.
- Intrinsic carrier concentration is the number of electron (=holes) per cubic centimeter populating the conduction band (or valence band) is called the intrinsic carrier concentration, n_i
- $n_i = f(T)$ that increases with increasing T (more thermal energy)

At Room Temperature (T=300 K)

$n_i \sim 2 \times 10^6 \text{ cm}^{-3}$ for GaAs with $E_g = 1.42 \text{ eV}$,

$n_i \sim 1 \times 10^{10} \text{ cm}^{-3}$ for Si with $E_g = 1.1 \text{ eV}$,

$n_i \sim 2 \times 10^{13} \text{ cm}^{-3}$ for Ge with $E_g = 0.66 \text{ eV}$,

$n_i \sim 1 \times 10^{-14} \text{ cm}^{-3}$ for GaN with $E_g = 3.4 \text{ eV}$

Clarification of confusing issues: “Holes” and Electrons

Terminology

Only these
“particles”
carry
electricity.
Thus, we
call these
“carriers”

Electrons: Sometimes referred to as conduction electrons: The electrons in the conduction band that are free to move throughout the crystal.

Holes: Missing electrons normally found in the valence band (or empty states in the valence band that would normally be filled).

If we talk about empty states in the conduction band, we DO NOT call them holes! This would be confusing. The conduction band has mostly empty states and a few electrons.

If we talk about filled states in the valence band, we DO NOT call them electrons! This would be confusing. We can call them Valence Electrons to indicate they are bond to atoms (in the valence shells of atoms). The valence band has mostly filled states and a few holes.

For the vast majority of this class we only talk about electrons (conduction band electrons) and holes (empty states in the valence band)!

Carrier Movement in Free Space

We must not only know how many electrons are present to conduct but we need to know how they move. For this we need to examine Newton's second law first in free space then in the crystal

Electrostatic force

Acceleration

$$F = -qE = m_o \frac{dv}{dt}$$

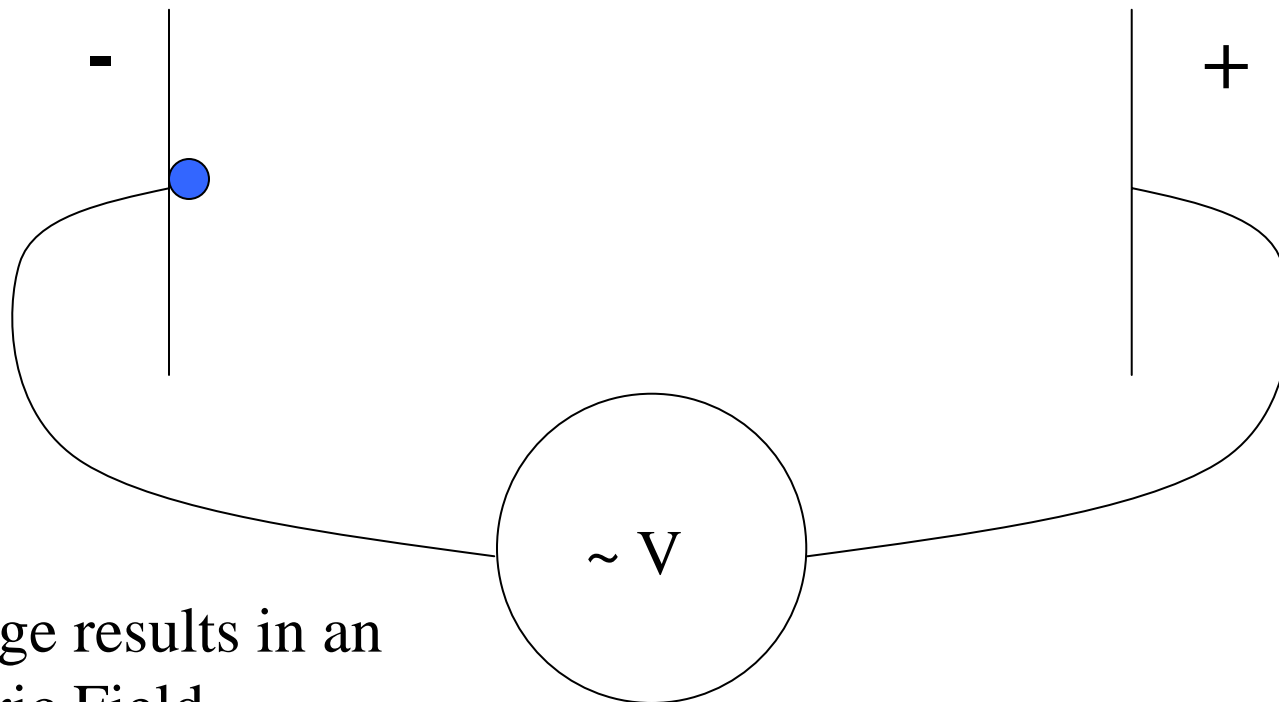
F ≡ force, *v* ≡ velocity, *t* ≡ time,

q ≡ electronic charge, *m_o* ≡ electron mass

Carrier Movement in Free Space vs a Crystal

What would happen to an electron if we could “magically” change it’s mass (physically we know this is not possible but what if) ?

Case One: Vacuum

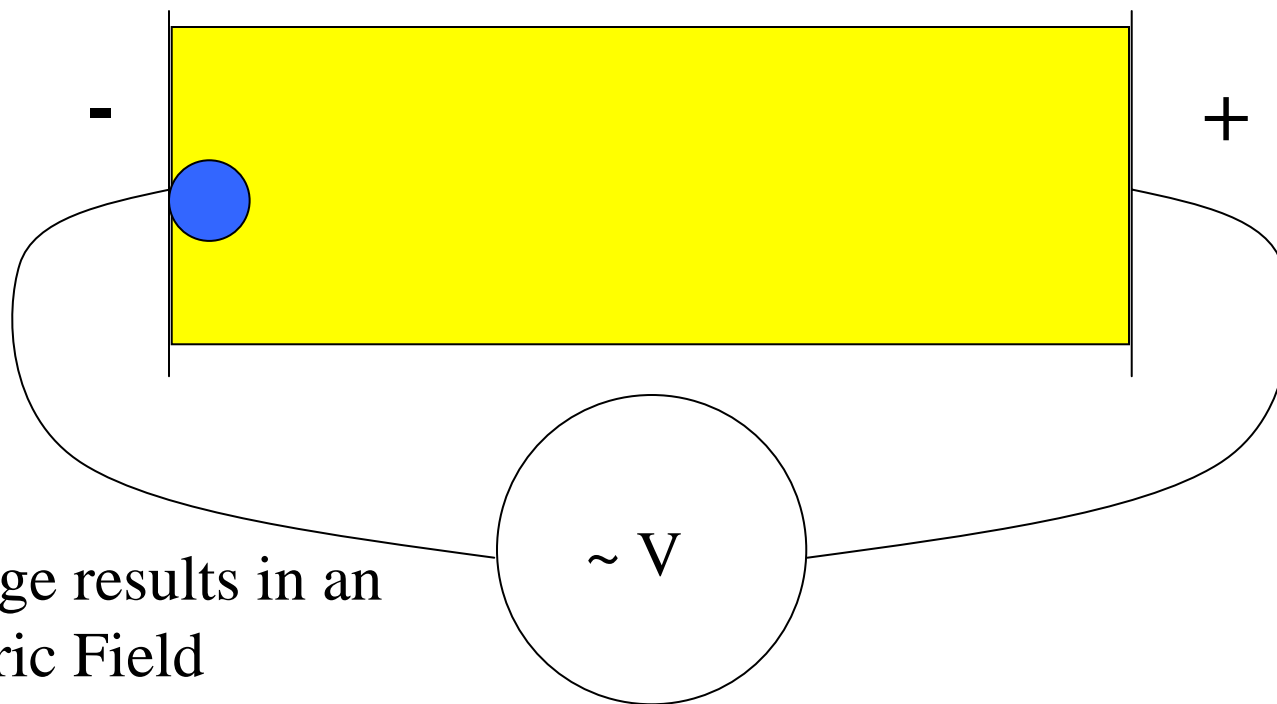


AC voltage results in an
AC electric Field

Carrier Movement in Free Space vs a Crystal

What would happen to an electron if we could “magically” change it’s mass (physically we know this is not possible but what if) ? ... It would respond to a high frequency AC electric field more sluggishly limiting the amount of current produced.

Case Two: Semiconductor with “larger electron mass”



AC voltage results in an
AC electric Field

Carrier Movement Within the Crystal

- While the actual mass does not change, the electrostatic effects of the crystal on the electron make it “appear” as if the electron had a different mass
- Electron is a quasi-particle that behaves as a “wave” due to quantum mechanical effects.
- The electron “wavelength” is perturbed by the crystals periodic potential.

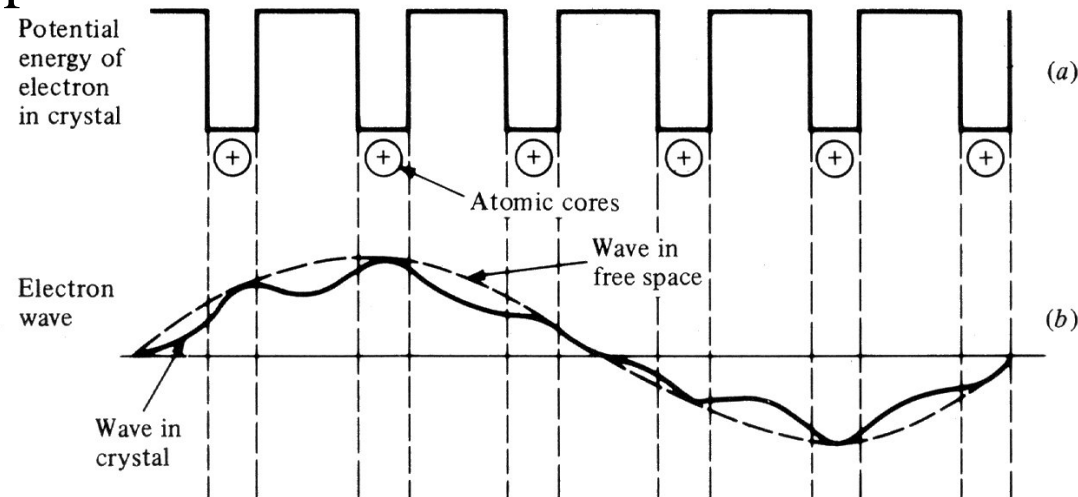
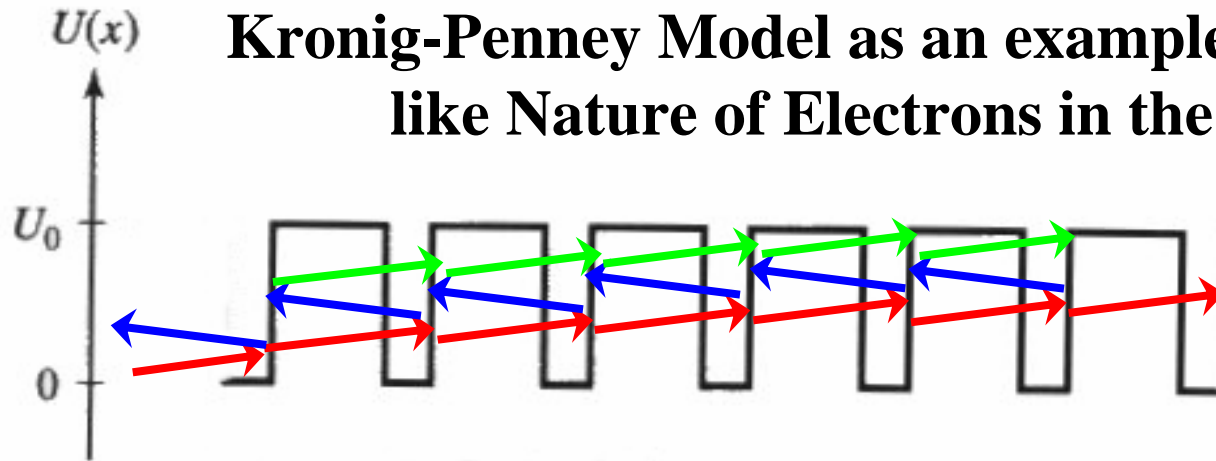


FIGURE 1-11
Representation of motion of electron wave in crystal potential. (After Wolfendale [3].)



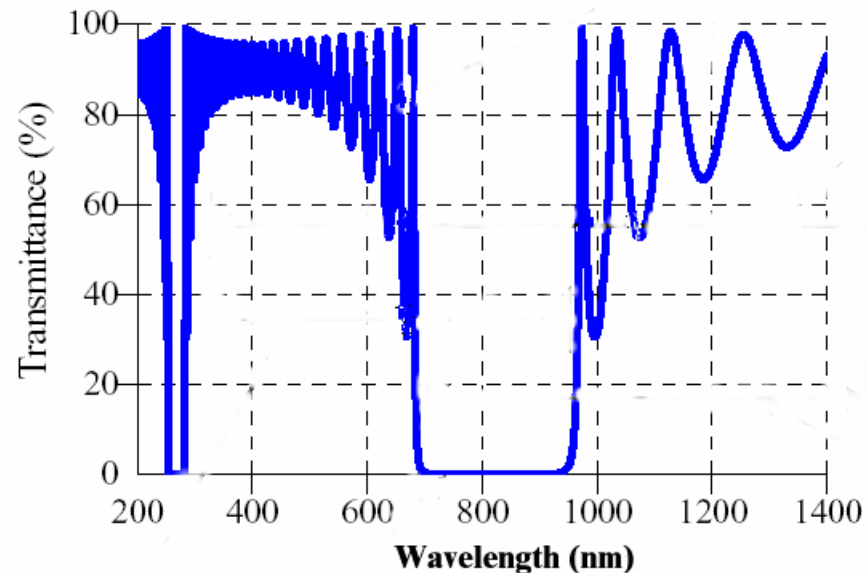
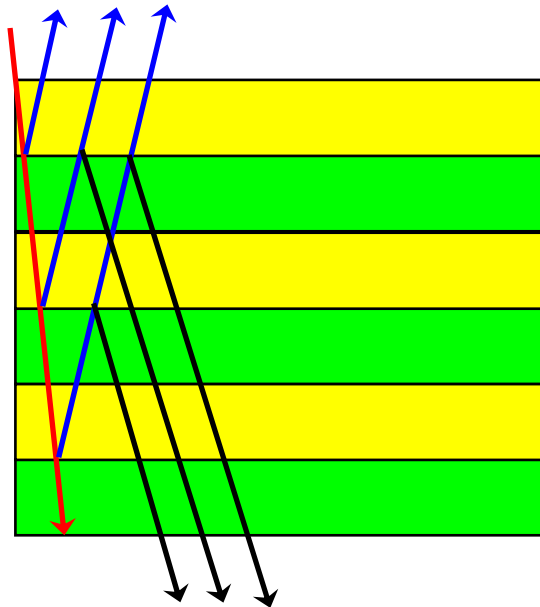
QuickTime Movie

Kronig-Penney Model as an example of the Wave-like Nature of Electrons in the Crystal



Resonant reflectance/transmission creates “standing waves” in the crystal. Only certain wavelengths (energies) can pass through the 1D crystal.

By analogy, a multiple layer optical coating has similar reflection/transmission characteristics. The result is the same, only certain wavelengths (energies) are transmitted through the optical stack. In a sense, we have an “optical bandgap”.



Carrier Movement Within the Crystal

We account for this complex interaction with the crystal (each crystal behaving differently) by using an “effective mass”

$$F = -qE = m_n^* \frac{dv}{dt}$$

$F \equiv$ force, $v \equiv$ velocity, $t \equiv$ time,

$q \equiv$ electronic charge,

$m_n^* \equiv$ electron effective mass

$$F = qE = m_p^* \frac{dv}{dt}$$

$F \equiv$ force, $v \equiv$ velocity, $t \equiv$ time,

$q \equiv$ electronic charge,

$m_p^* \equiv$ hole effective mass

Table 2.1 Density of States Effective Masses at 300 K.

Material	m_n^*/m_0	m_p^*/m_0
Si	1.18	0.81
Ge	0.55	0.36
GaAs	0.066	0.52

Ge and GaAs have “lighter electrons” than Si
which results in faster devices

The need for more control over carrier concentration

Without “help” the total number of “carriers” (electrons and holes) is limited to $2n_i$.

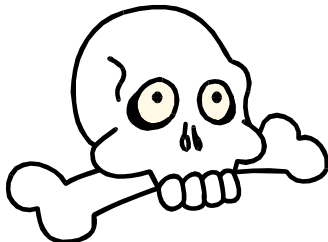
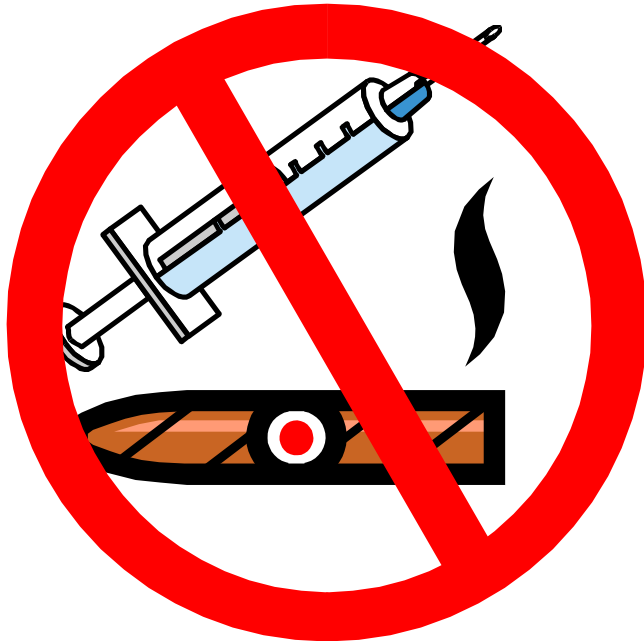
For most materials, this is not that much, and leads to very high resistance and few useful applications.

We need to add carriers by modifying the crystal.

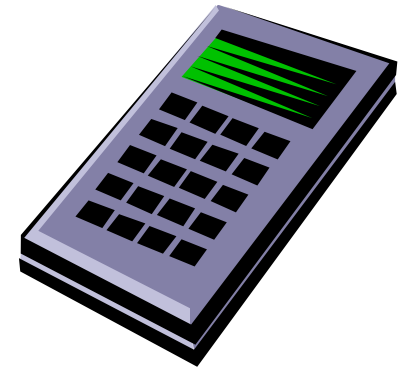
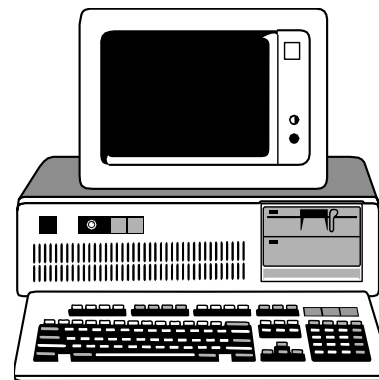
This process is known as “doping the crystal”.

Regarding Doping, ...

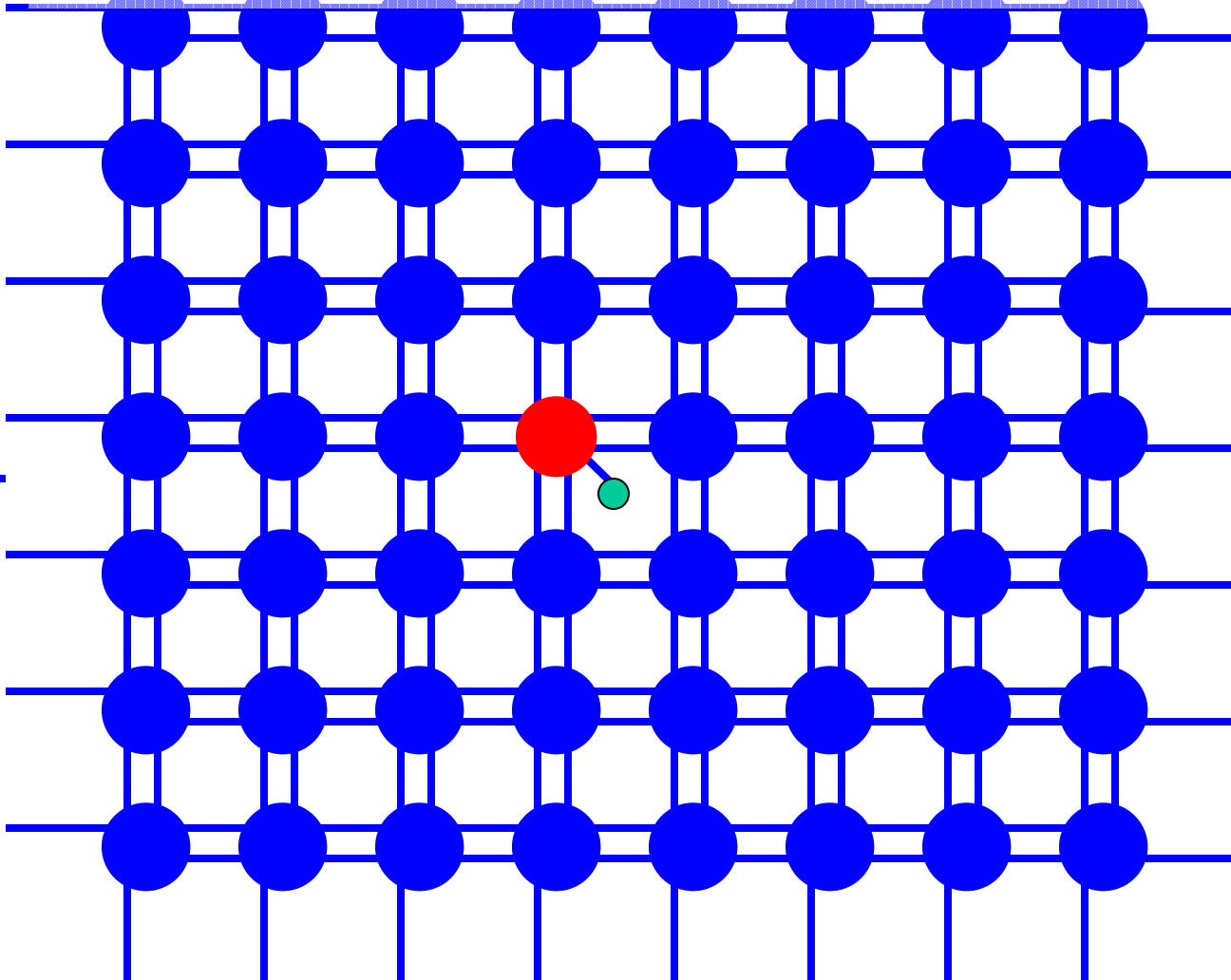
Just Say No!



**Just Say Yes
to Crystal Doping!**



Extrinsic, (or doped material): Concept of a Donor “adding extra” electrons



Example:
P, As, Sb
in Si

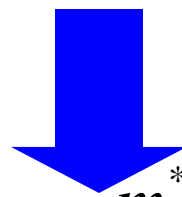
Concept of a Donor “adding extra” electrons

Use the Hydrogen Atomic Energy levels to approximate the energy required to free an electron on a donor.

- Replace dielectric constant with that of the semiconductor
- Replace mass with that of the semiconductor

$$\text{Energy}_{\text{Hydrogen electron}} = E_H = -\frac{m_o q^4}{2(4\pi\epsilon_o \hbar n)^2} = -\frac{13.6 \text{ eV}}{n^2}$$

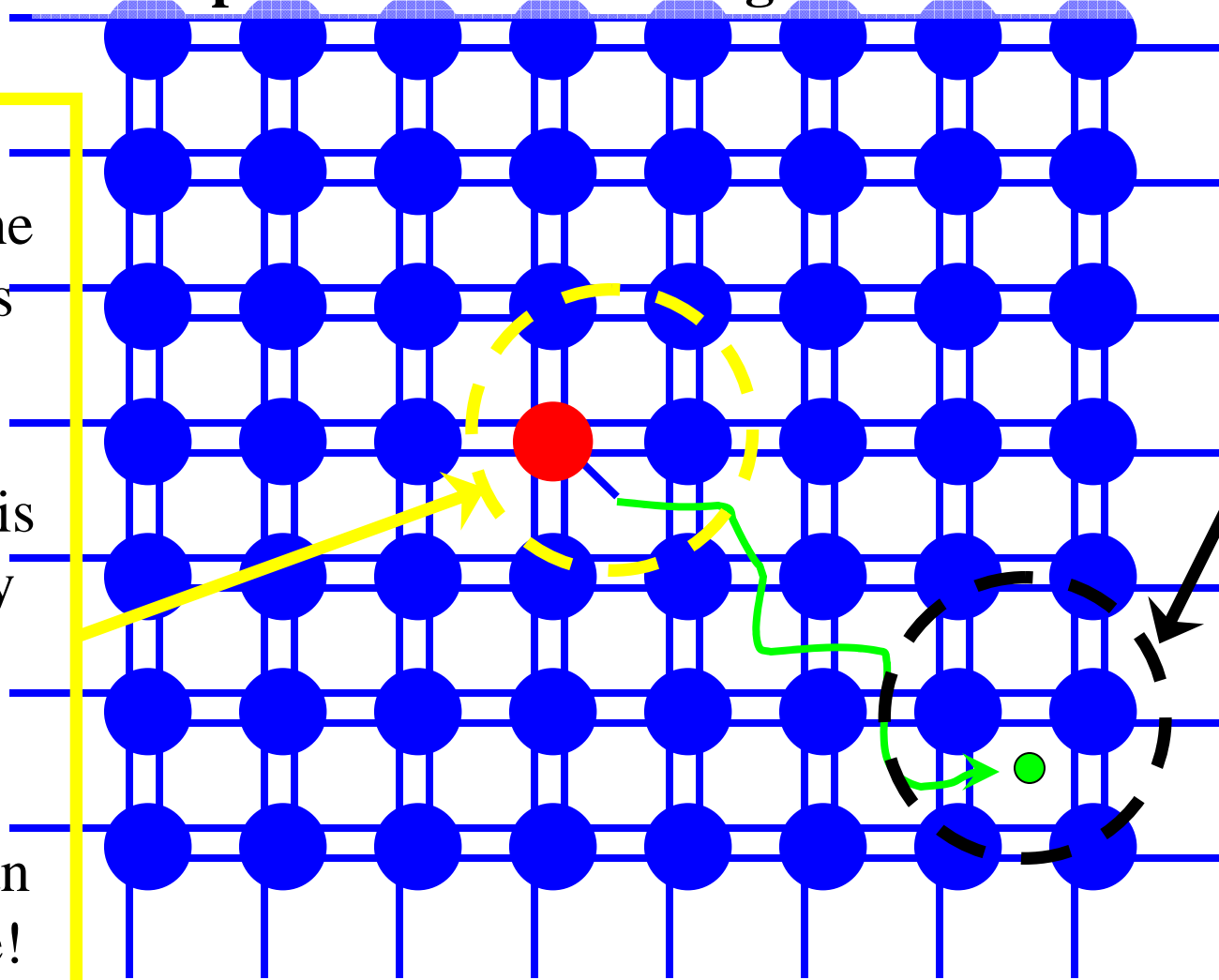
where m_o = electron mass, \hbar = planks constant / $2\pi = h / 2\pi$
 q = electron charge, and $n = 1, 2, 3, \dots$



$$E_{\text{Binding for electron}} \approx -\frac{m_n^* q^4}{2(4\pi\epsilon_R \epsilon_o \hbar n)^2} = \frac{m_n^*}{m_o} \frac{1}{\epsilon_R^2} E_H \cong -0.1 \text{ eV for } n = 1$$

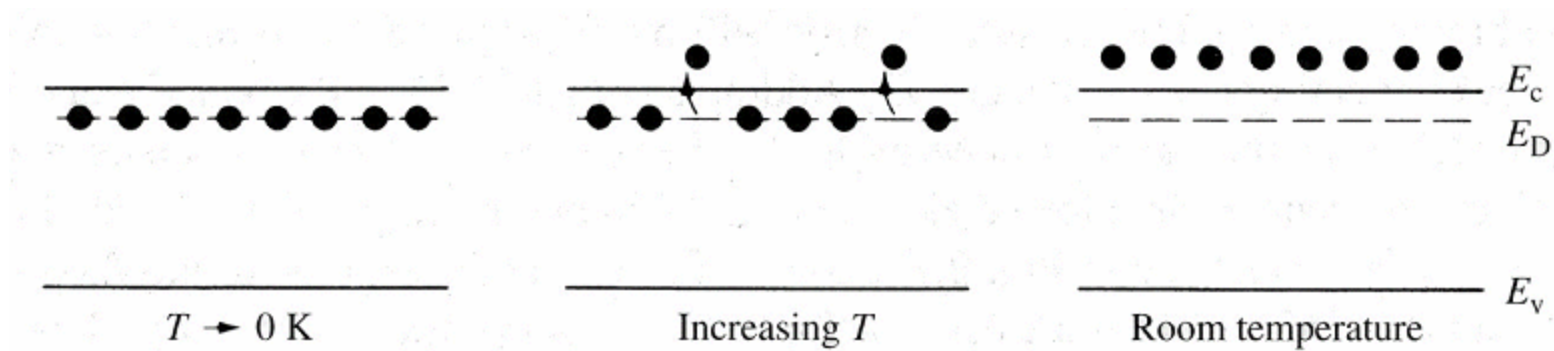
Extrinsic, (or doped material): Concept of a Donor “adding extra” electrons

Region around the donor has one less electron and thus is positively charged. This charged region can not move!

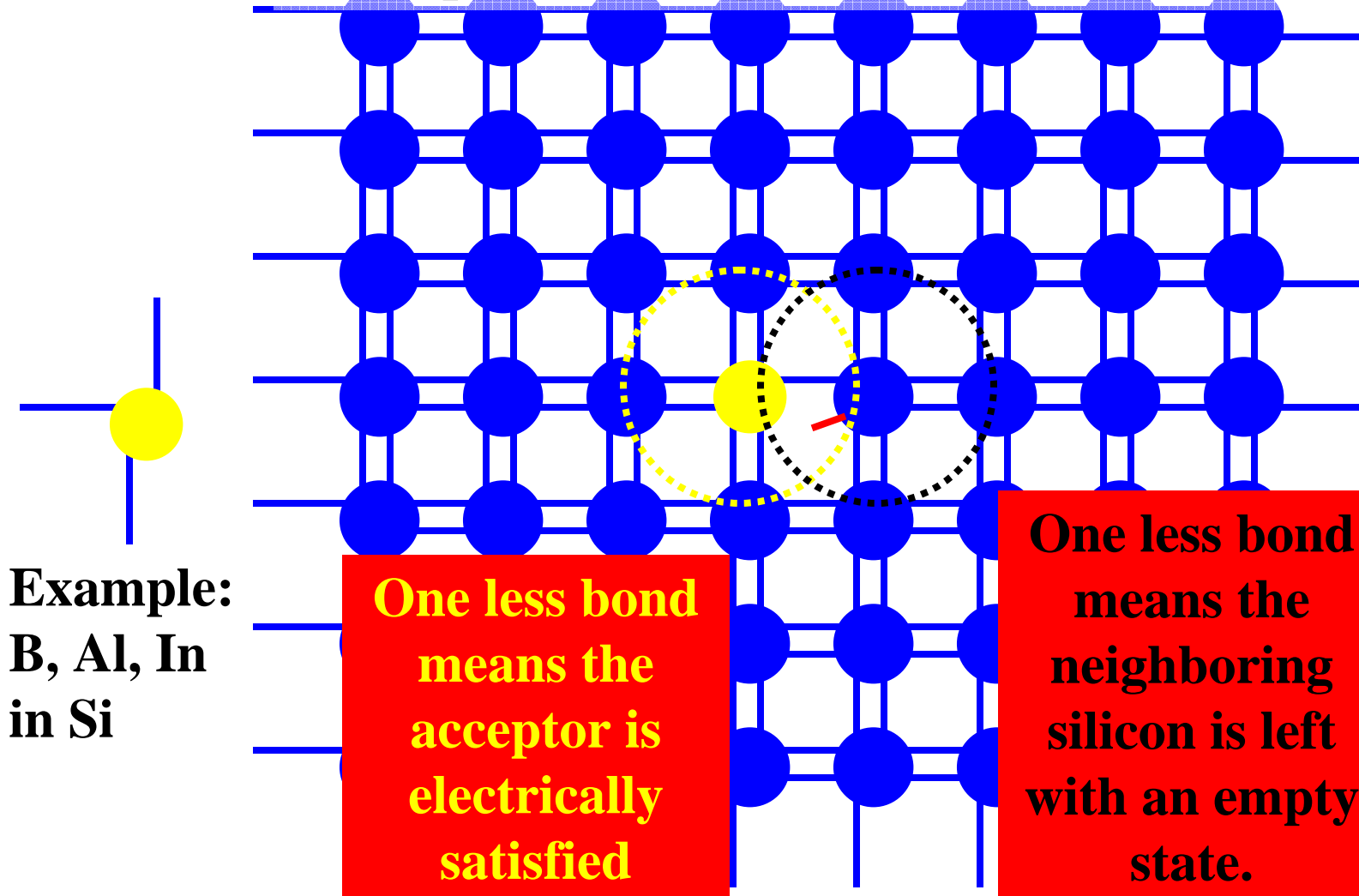


Region around the electron has one more electron and thus is negatively charged. The electron can move.

Concept of a Donor “adding extra” electrons: Band diagram equivalent view



**Extrinsic, (or doped material):
Concept of an acceptor “adding extra” holes**



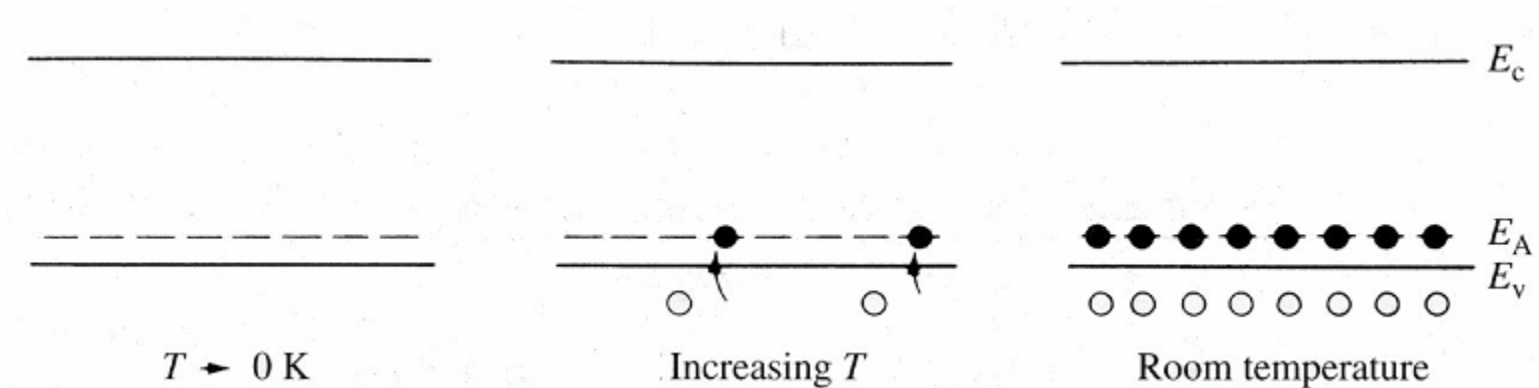
All regions of material are neutrally charged.

**Example:
B, Al, In
in Si**

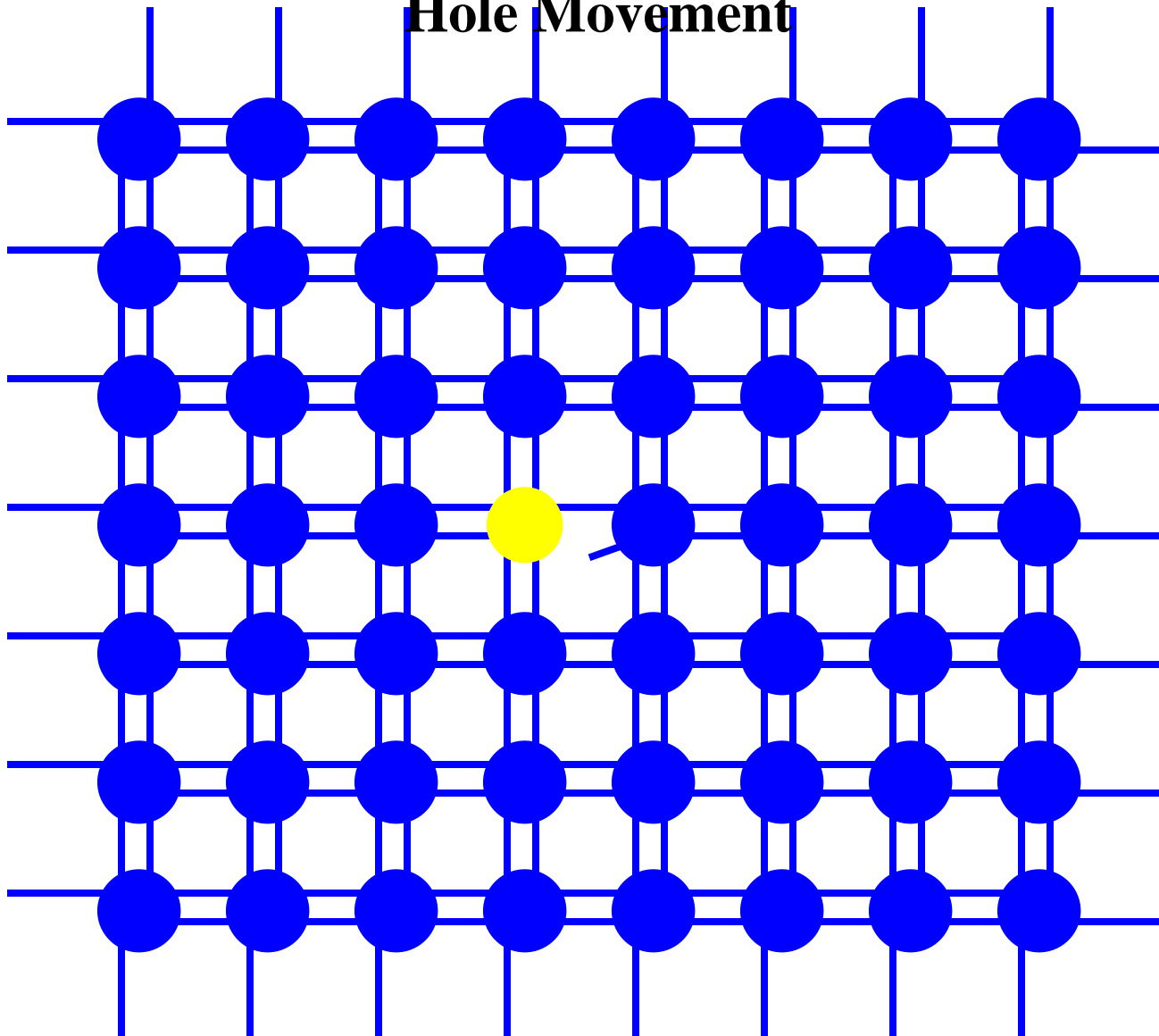
One less bond means the acceptor is electrically satisfied

One less bond means the neighboring silicon is left with an empty state.

Concept of an Acceptor “adding extra hole”: Band diagram equivalent view



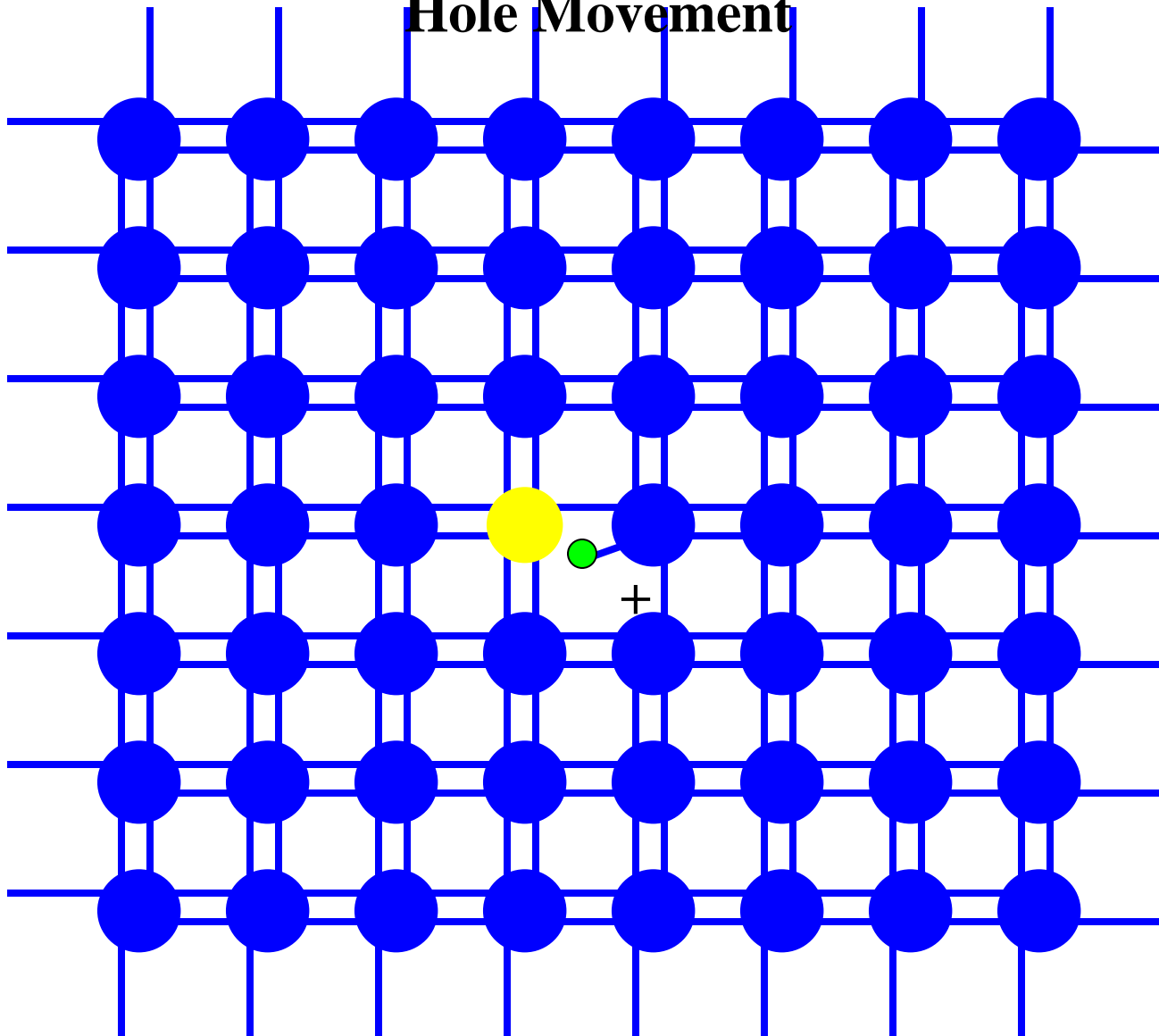
Hole Movement



All regions of material are neutrally charged.

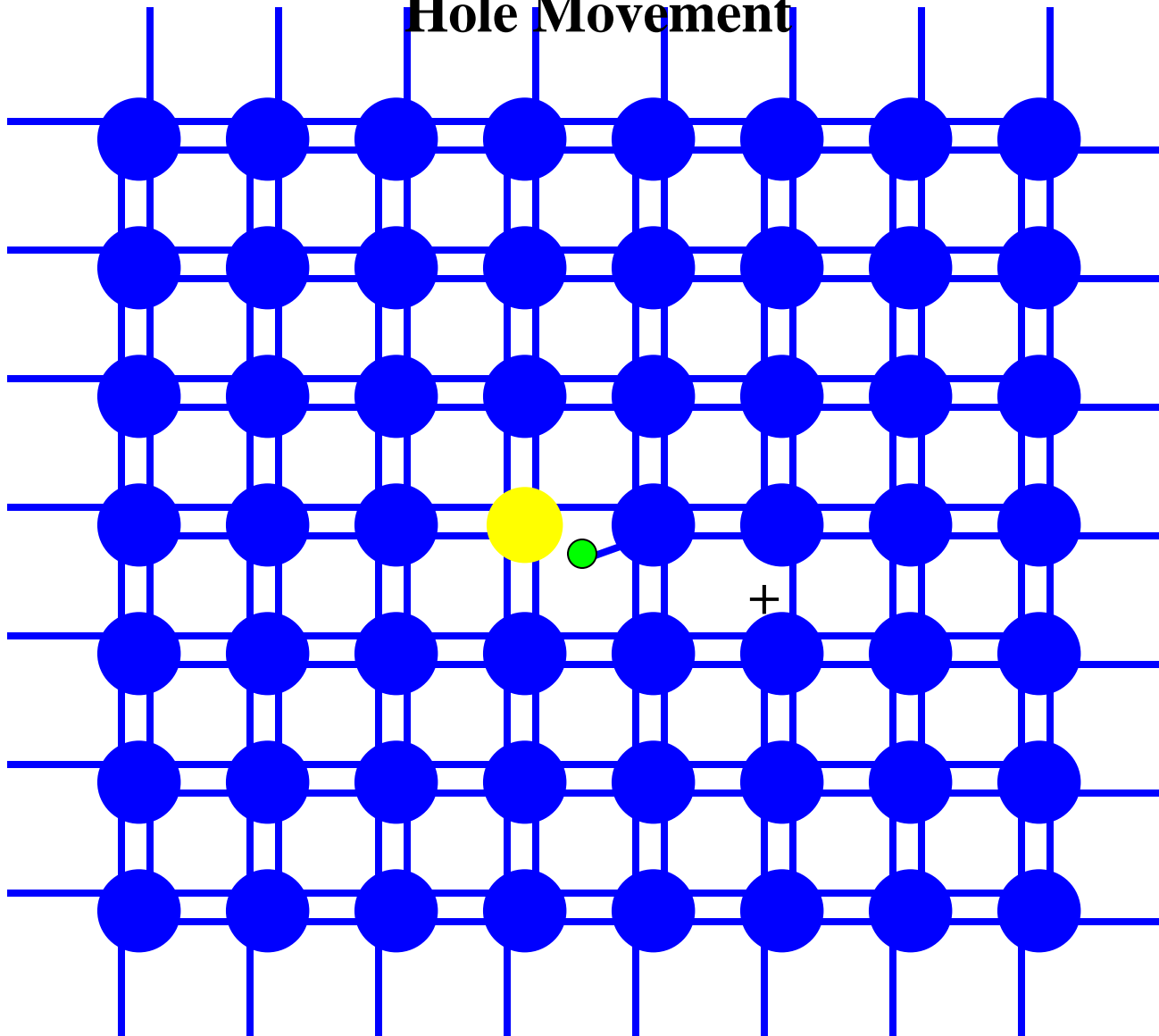
Empty state is located next to the Acceptor

Hole Movement



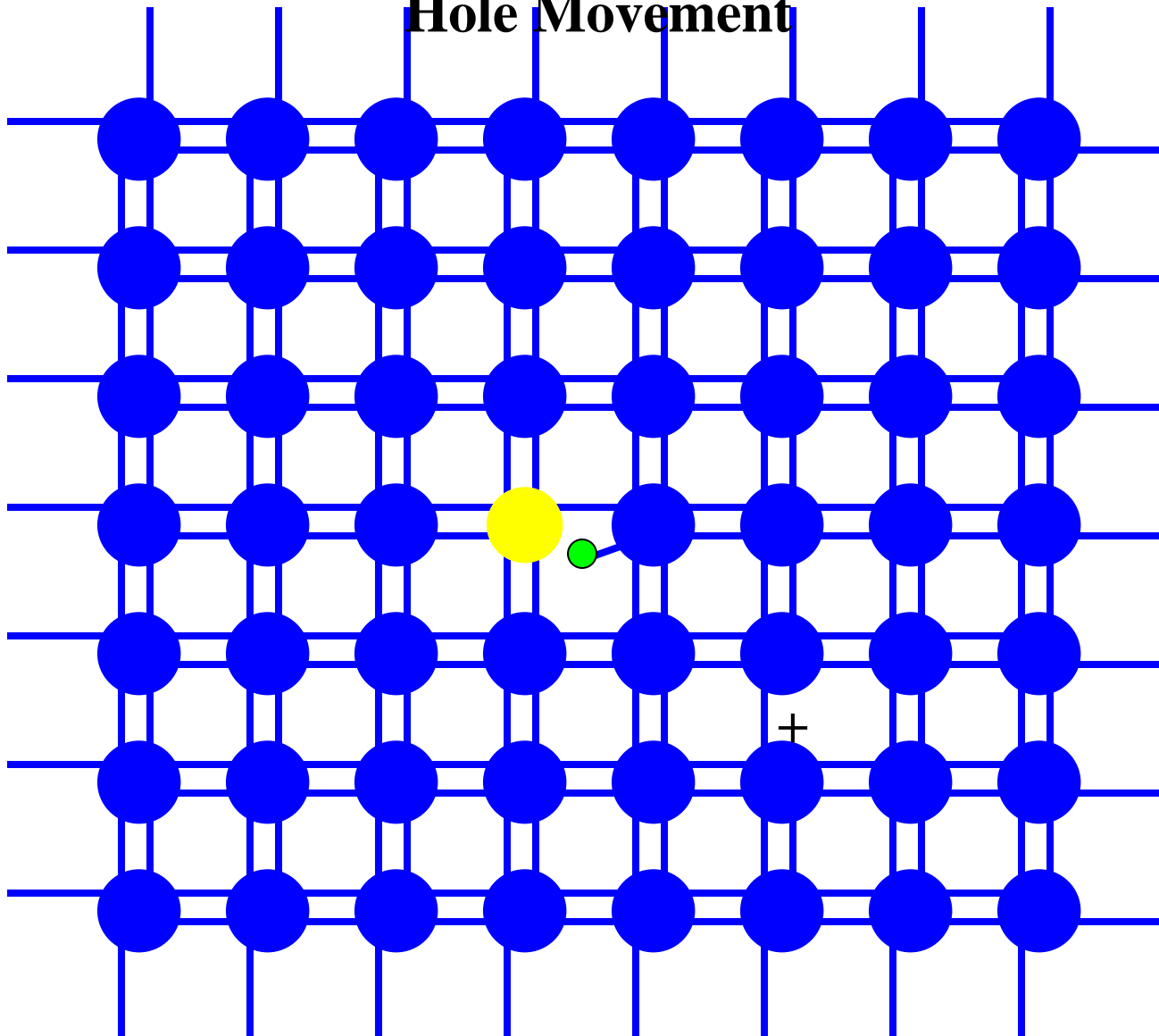
Another valence electron can fill the empty state located next to the Acceptor leaving behind a positively charged “hole”.

Hole Movement



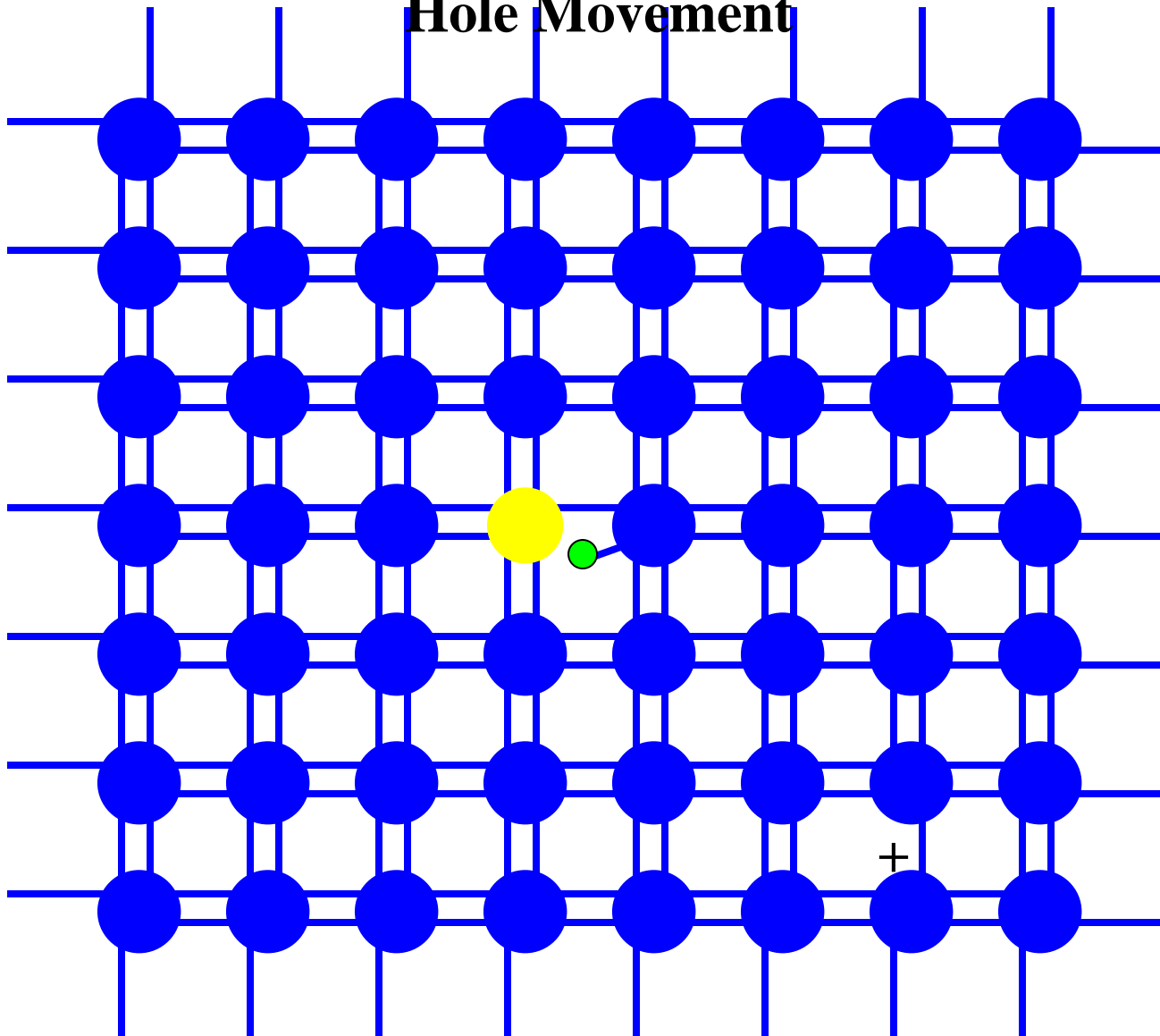
The positively charged “hole” can move throughout the crystal
(really it is the valance electrons jumping from atom to atom that creates the hole motion).

Hole Movement



The positively charged “hole” can move throughout the crystal
(really it is the valance electrons jumping from atom to atom that creates the hole motion).

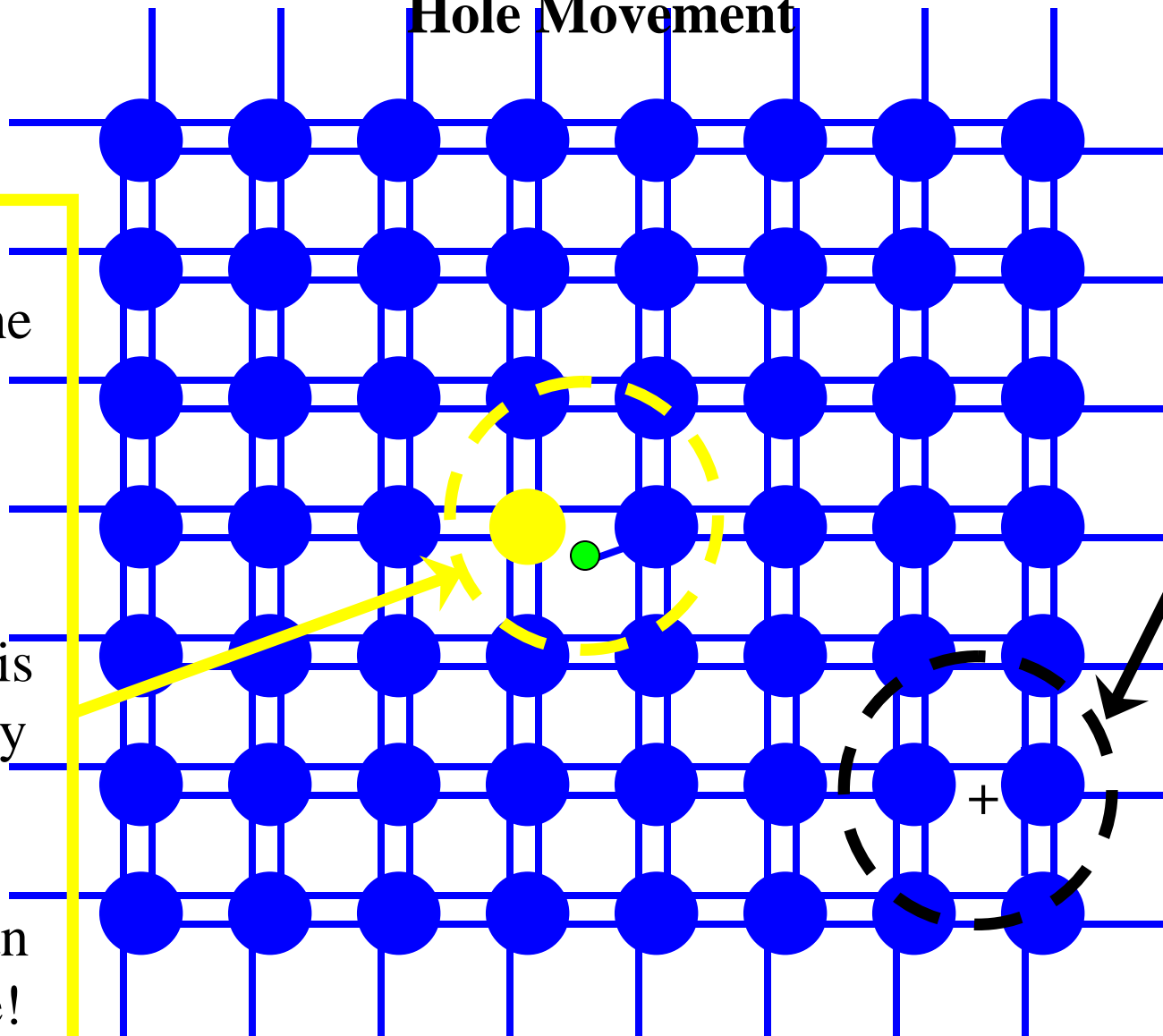
Hole Movement



The positively charged “hole” can move throughout the crystal
(really it is the valance electrons jumping from atom to atom that creates the hole motion).

Hole Movement

Region around the acceptor has one extra electron and thus is negatively charged. This region can not move!



Region around the "hole" has one less electron and thus is positively charged. The hole can move!

The positively charged "hole" can move throughout the crystal

(really it is the valance electrons jumping from atom to atom that creates the hole motion).

Summary of Important terms and symbols

Bandgap Energy: Energy required to remove a valence electron and allow it to freely conduct.

Intrinsic Semiconductor: A “native semiconductor” with no dopants. Electrons in the conduction band equal holes in the valence band. The concentration of electrons (=holes) is the intrinsic concentration, n_i .

Extrinsic Semiconductor: A doped semiconductor. Many electrical properties controlled by the dopants, not the intrinsic semiconductor.

Donor: An impurity added to a semiconductor that adds an additional electron not found in the native semiconductor.

Acceptor: An impurity added to a semiconductor that adds an additional hole not found in the native semiconductor.

Dopant: Either an acceptor or donor.

N-type material: When electron concentrations (n =number of electrons/cm³) exceed the hole concentration (normally through doping with donors).

P-type material: When hole concentrations (p =number of holes/cm³) exceed the electron concentration (normally through doping with acceptors).

Majority carrier: The carrier that exists in higher population (ie n if $n > p$, p if $p > n$)

Minority carrier: The carrier that exists in lower population (ie n if $n < p$, p if $p < n$)

Other important terms (among others): Insulator, semiconductor, metal, amorphous, polycrystalline, crystalline (or single crystal), lattice, unit cell, primitive unit cell, zincblende, lattice constant, elemental semiconductor, compound semiconductor, binary, ternary, quaternary, atomic density, Miller indices, various notations, etc...