Chapter 2

SEMICONDUCTOR BANDSTRUCTURE

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 ~10^{23} atoms 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.

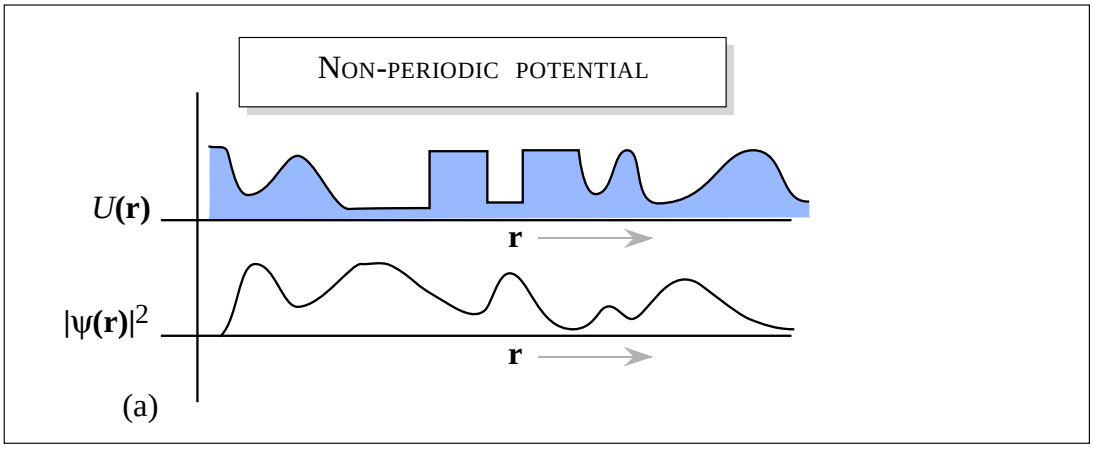
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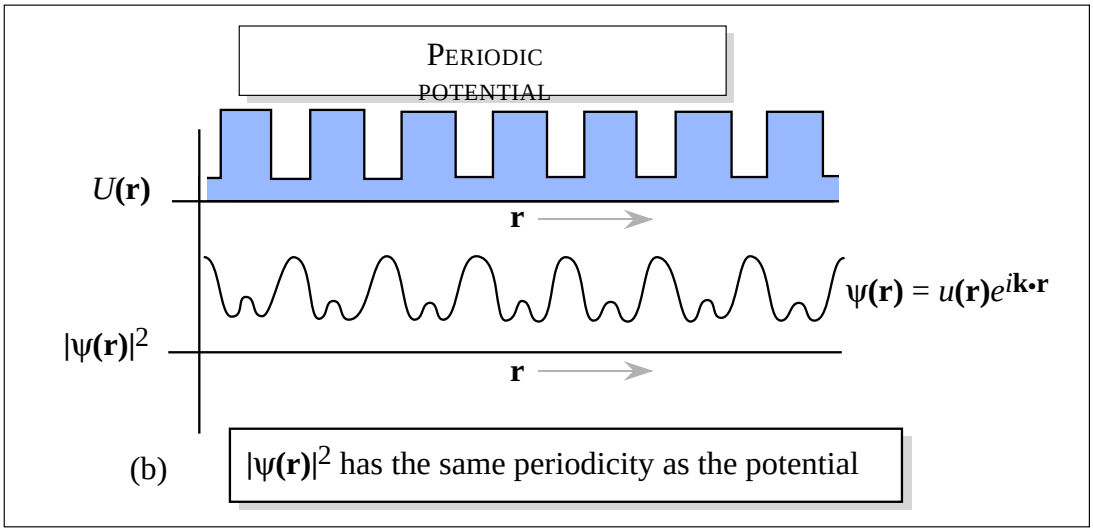
BLOCH THEOREM:

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.

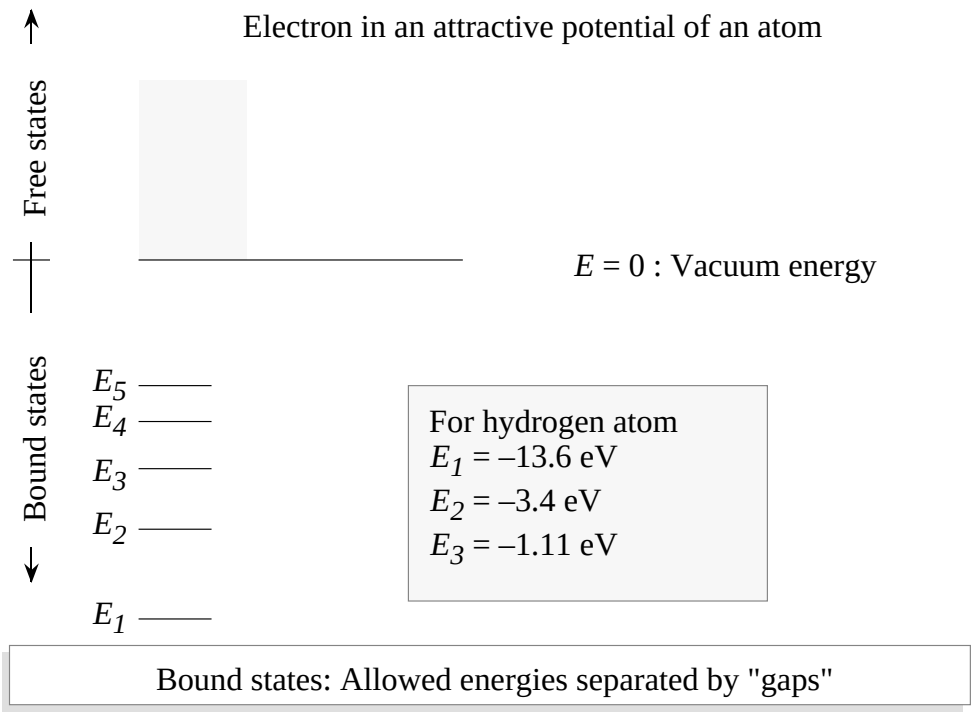
k is called the crystal momentum.

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

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ELECTRONS IN AN ATOM

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



Allowed energy levels:

$$E_n = \frac{-me^4}{2(4\pi\varepsilon_0)^2\hbar^2 n^2} = \frac{-13.6}{n^2} \text{ eV}$$

Wavefunctions:

$\psi_{n\ell m}$: n: principle quantum number.

ℓ: orbital quantum number; angular momentun of the electron = $\ell\hbar$, ℓ = 0, 1, 2...

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

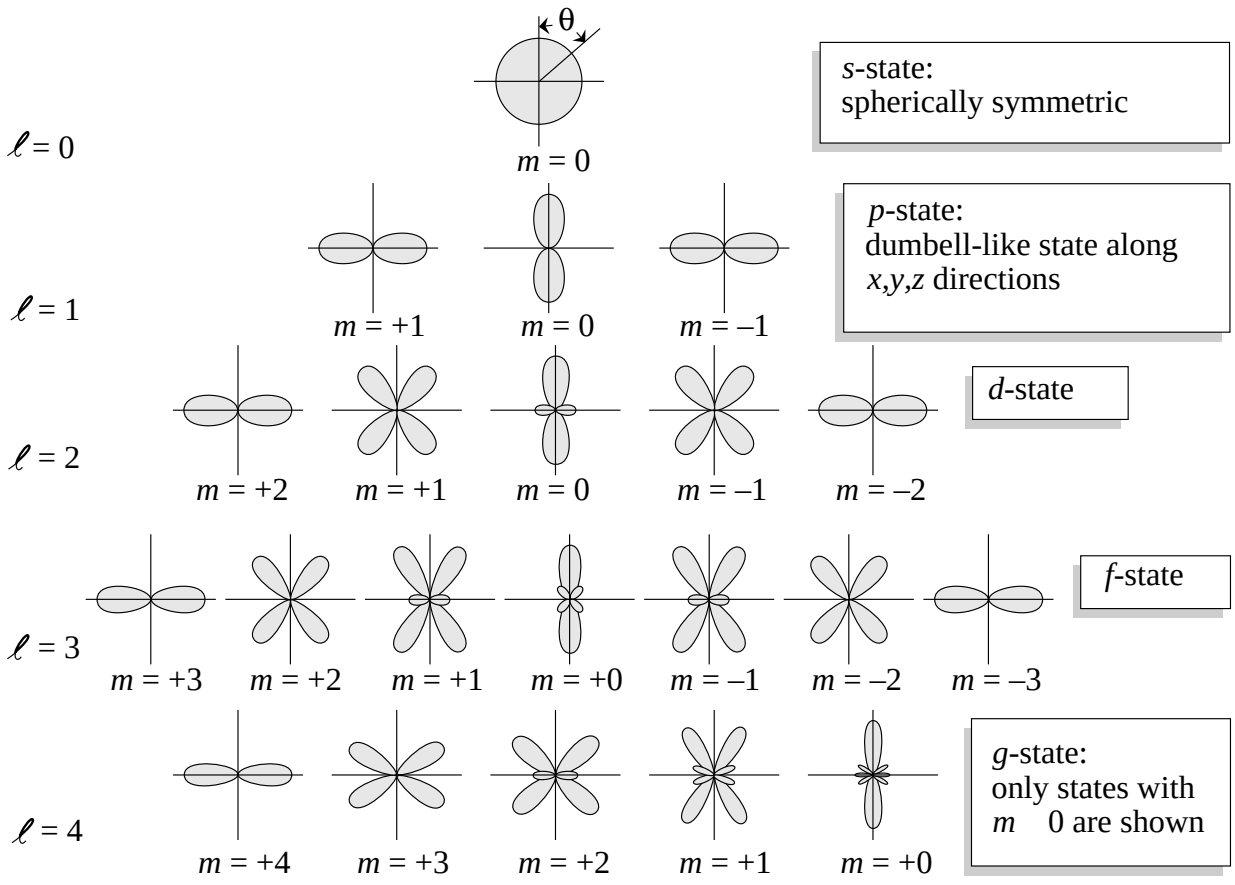
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NATURE OF ATOMIC FUNCTIONS:

These are important, since the cell periodic part of Block states is often made up of atomic-like states

ℓ=0: angular momentum is zero; called *s*-state

ℓ=1: angular momentum is one ($\hbar$); called *p*-state

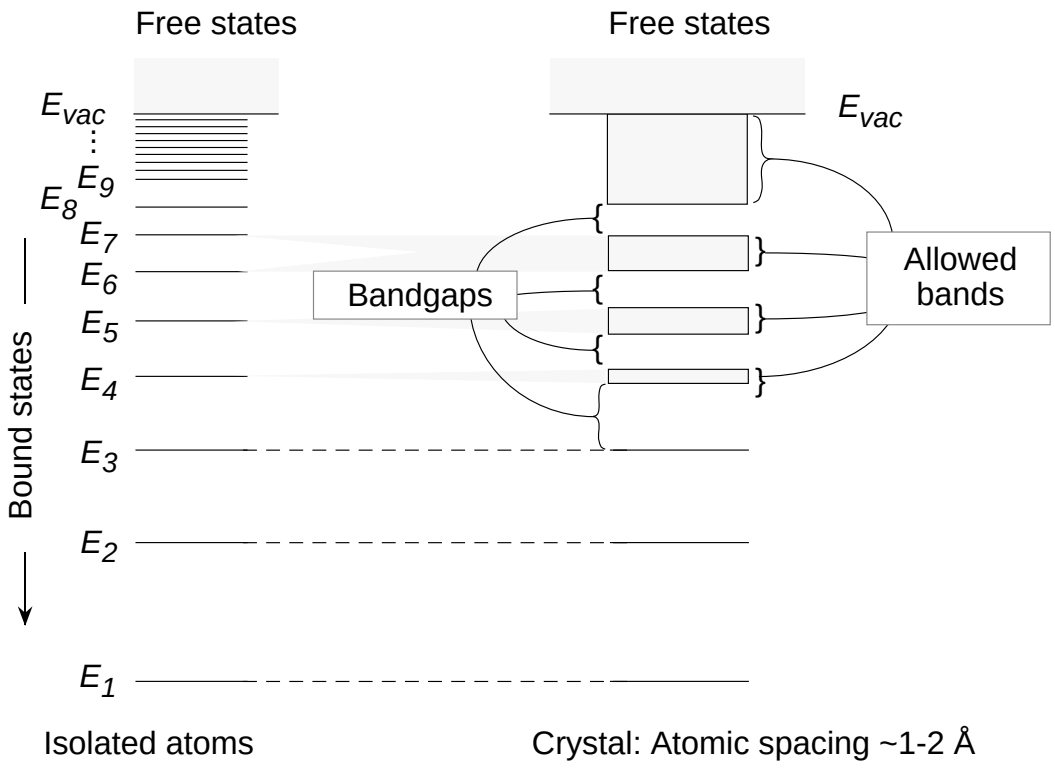


A plot of the probability density function of electronic states in an atom as a function of the angle θ for the
s, p, d, f, g electrons.

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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 (~$e^{i\mathbf{k}\bullet\mathbf{r}}$).



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

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SEMICONDUCTOR BANDSTRUCTURE

In semiconductors we are pimarily interested in the valence band and conduction band. Moreover, for most applications we are interested in what happens near the top of the valence band and the bottom of the conduction band. These states originate from the atomic levels of the valence shell in the elements making up the semiconductor.

IV Semiconductors

C $1s^2\underbrace{2s^2 2p^2}$

Si $1s^2 2s^2 2p^6 \underbrace{3s^2 3p^2}$

Ge $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} \underbrace{4s^2 4p^2}$

III-V Semiconductors

Ga $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} \underbrace{4s^2 4p^1}$

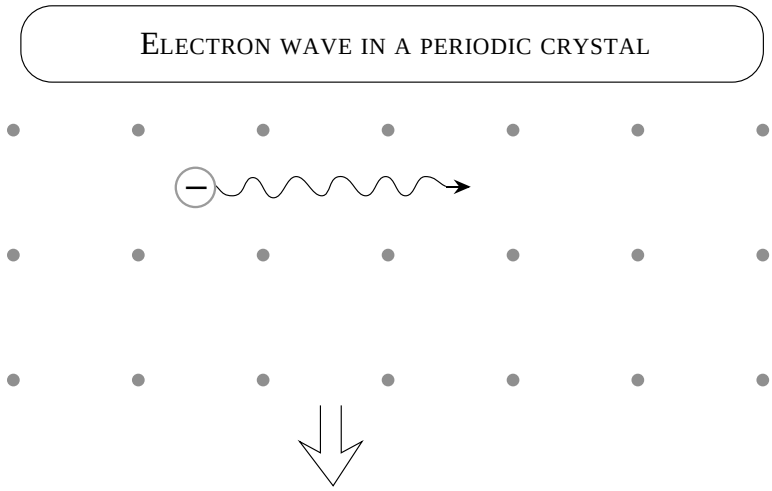
As $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} \underbrace{4s^2 4p^3}$

Outermost atomic levels are either *s*-type or *p*-type.

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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^*.



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:	$\frac{\hbar dk}{dt}$ = Force $E = \frac{\hbar^2 k^2}{2m^*}$

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BANDSTRUCTURE OF SEMICONDUCTORS

The *k*-vector for the electrons in a crystal is limited to a space called the Brillouin zone. The figure shows the Brillouin zone for the fcc lattice relevant for most semiconductors. The values and notations of certain important *k*-points are also shown. Most semiconductors have bandedges of allowed bands at one of these points.

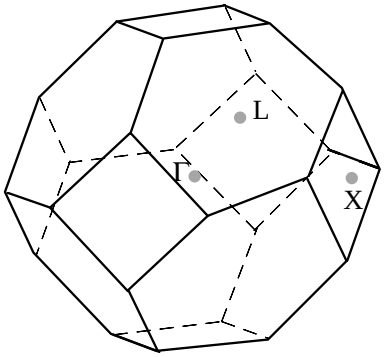
IMPORTANT HIGH SYMMETRY POINTS

Γ point: $k_x = 0 = k_y = k_z$

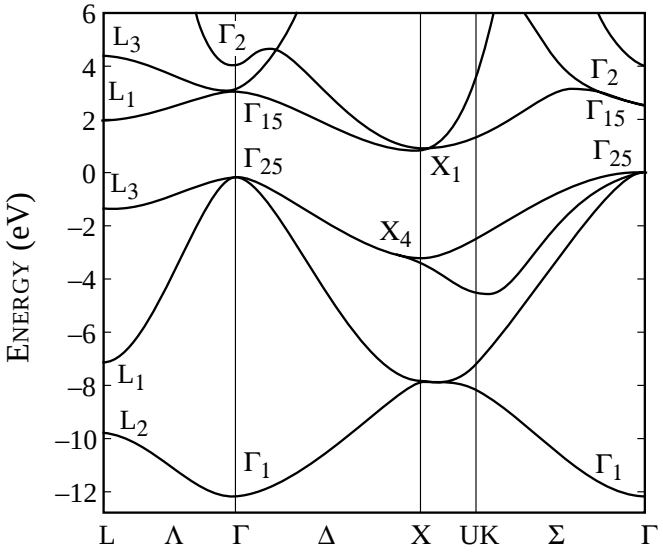
X point: $k_x = \frac{2\pi}{a}$; $k_y = k_z = 0$

L point: $k_x = k_y = k_z = \frac{\pi}{a}$

a = lattice constant (cube edge)



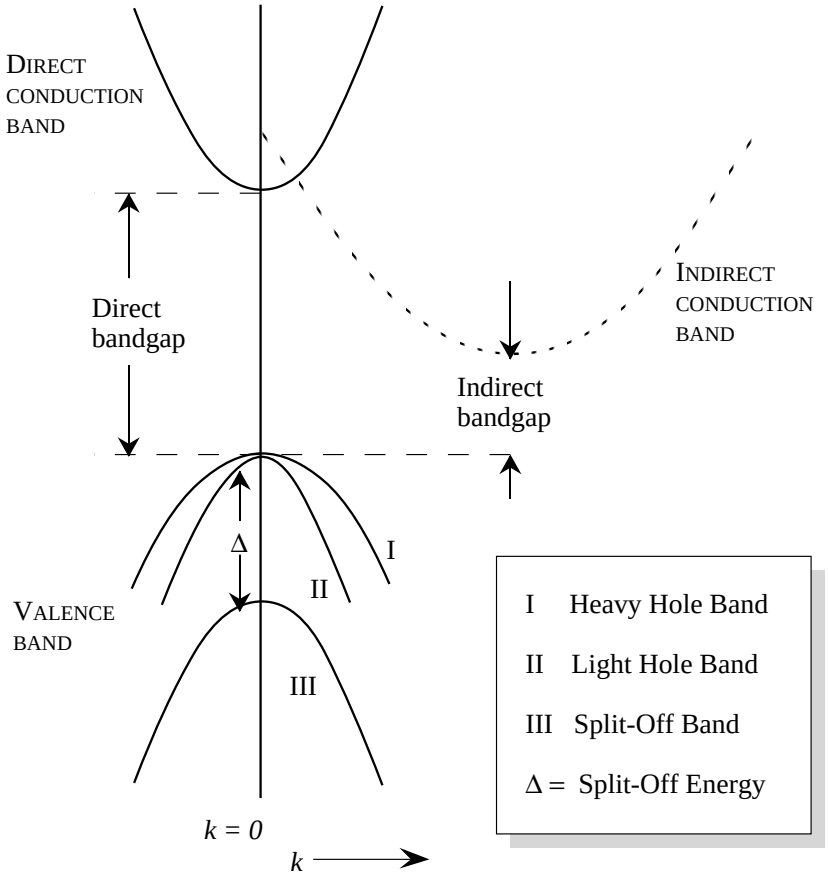
A TYPICAL BANDSTRUCTURE: Si



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BANDSTRUCTURE NEAR BANDEDGES

Behavior of electrons near the bandedges determines most device properties. Near the bandedges the electrons can be described by simple effective mass pictures, i.e., the electrons behave as if they are in free space except their masses are *m**.



Schematic of the valence band, direct bandgap, and indirect bandgap conduction bands. The conduction band of the direct gap semiconductor is shown in the solid line, while the conduction band of the indirect semiconductor is shown in the dashed line. The curves I, II, and III in the valence band are called *heavy hole, light hole, and split-off hole states*, respectively.

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EFFECTIVE MASS DESCRIPTION

CONDUCTION BAND: Direct bandgap material

$$E_c(\boldsymbol{k}) = E_c(0) + \frac{\hbar^2 k^2}{2m_c^*}$$

with

$$\frac{1}{m_c^*} = \frac{1}{m_0} + \frac{2p_{cv}^2}{m_0^2}\frac{1}{3}\left(\frac{2}{E_{g\Gamma}} + \frac{1}{E_{g\Gamma}+\Delta}\right); \quad \frac{2p_{cv}^2}{m_0} \sim 22 \text{ eV}$$

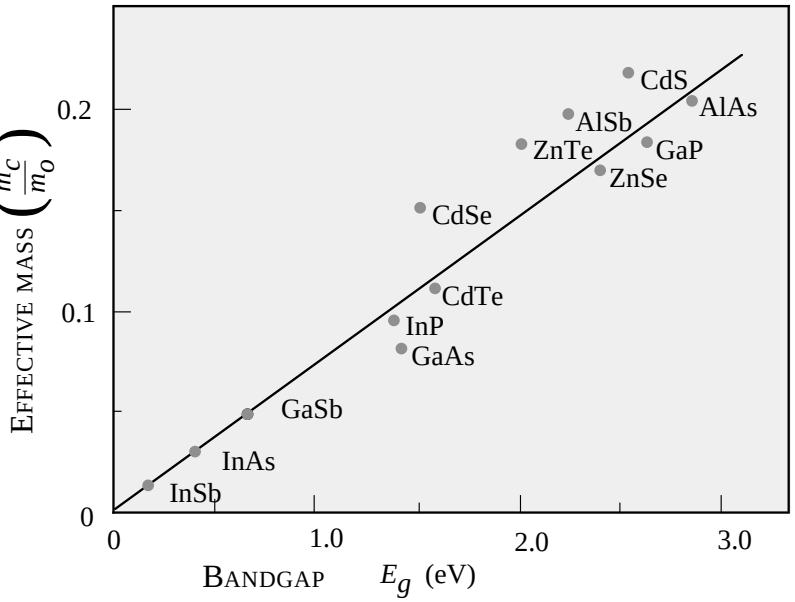
The smaller the bandgap, the smaller the effective mass.

SPLIT-OFF BAND:

$$E_{so} = -\Delta - \frac{\hbar^2 k^2}{2m_{so}^*}$$

$$\frac{1}{m_{so}^*} = \frac{-1}{m_0} + \frac{2p_{cv}^2}{3m_0^2(E_{g\Gamma}+\Delta)}$$

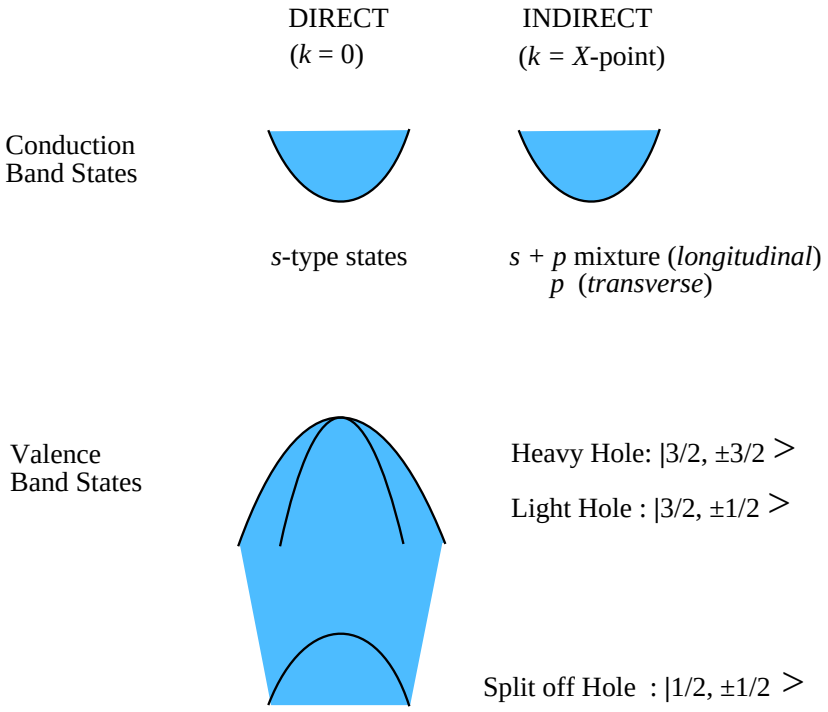
HEAVY HOLE; LIGHT HOLE:
In a simple approximation the heavy hole and light hole bands can also be represented by masses m^*_{hh} and m^*_{lh}. However, the real picture is more complex.



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CHARACTER OF THE WAVEFUNCTIONS NEAR THE BANDEDGES

The wavefunction (central cell) determines the nature of optical transistion in optoelectronic devices.



Top of the valence band is made from *p*-type states. Combining spin, the total angular momentum of the states is 3/2$\hbar$.

$$\Phi_{3/2,3/2} = \frac{-1}{\sqrt{2}}\,(|p_x> + i|p_y>)\uparrow$$

$$\Phi_{3/2,-3/2} = \frac{-1}{\sqrt{2}}\,(|p_x> - i|p_y>)\downarrow$$

$$\Phi_{3/2,1/2} = \frac{-1}{\sqrt{6}}\,[(|p_x> + i|p_y>)\downarrow - 2|p_z>\uparrow]$$

$$\Phi_{3/2,-1/2} = \frac{1}{\sqrt{6}}\,[(|p_x> - i|p_y>)\uparrow + 2|p_z>\downarrow]$$

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6 BAND k•p THEORY FOR THE VALENCE BAND

j:	3/2	3/2	3/2	3/2	1/2	1/2
m_j:	3/2	1/2	–1/2	–3/2	1/2	–1/2

$$H = -\begin{bmatrix} H_{hh} & b & c & 0 & ib/\sqrt{2} & -i/\sqrt{2}c \\ b^* & H_{lh} & 0 & c & -iq & i\sqrt{3}b/\sqrt{2} \\ c^* & 0 & H_{lh} & -b & i\sqrt{3}b^*/\sqrt{2} & -iq \\ 0 & c^* & -b^* & H_{hh} & -i\sqrt{2}c^* & -ib^*/\sqrt{2} \\ -ib^*/\sqrt{2} & iq & i\sqrt{3}b/\sqrt{2} & i\sqrt{2}c & H_{so} & 0 \\ i/\sqrt{2}c^* & -i\sqrt{3}b^*/\sqrt{2} & iq & ib/\sqrt{2} & 0 & H_{so} \end{bmatrix}$$

6-band

The elements in the Hamiltonian are given by

$$H_{hh} = \frac{\hbar^2}{2m_0}\left[\{(\gamma_1+\gamma_2)(k_x^2+k_y^2)+(\gamma_1-2\gamma_2)k_z^2\right]$$

$$H_{lh} = \frac{\hbar^2}{2m_0}\left[\{(\gamma_1-\gamma_2)(k_x^2+k_y^2)+(\gamma_1+2\gamma_2)k_z^2\right]$$

$$H_{so} = (H_{hh}+H_{lh})/2+\Delta_0$$

$$b = \frac{-\sqrt{3}i\hbar^2}{m_0}\gamma_3(k_x-ik_y)k_z$$

$$c = \frac{\sqrt{3}\hbar^2}{2m_0}\left[\gamma_2(k_x^2-k_y^2)-2i\gamma_3k_xk_y\right]$$

$$q = (H_{hh}-H_{lh})/\sqrt{2}$$

In most semiconductors with large spin-orbit coupling, the 6 x 6 matric equation can be separated into a 4 x 4 and a 2 x 2 equation. The appropriate equation defining the HH and LH states is then

4-band

$$-\begin{bmatrix} H_{hh} & b & c & 0 \\ b^* & H_{lh} & 0 & c \\ c^* & 0 & H_{lh} & -b \\ 0 & c^* & -b^* & H_{hh} \end{bmatrix}\begin{bmatrix} \Phi_{(3/2,3/2)} \\ \Phi_{(3/2,1/2)} \\ \Phi_{(3/2,-1/2)} \\ \Phi_{(3/2,-3/2)} \end{bmatrix} = E\begin{bmatrix} \Phi_{(3/2,3/2)} \\ \Phi_{(3/2,1/2)} \\ \Phi_{(3/2,-1/2)} \\ \Phi_{(3/2,-3/2)} \end{bmatrix}$$

A further transformation can be done to reduce the problem:

2-band

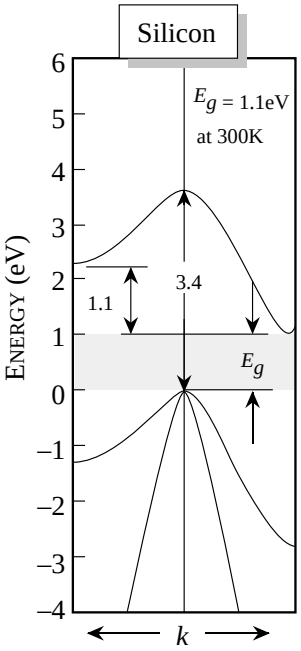
$$\begin{vmatrix} H_{hh} & |b|-i|c| \\ (|b|-i|c|)^* & H_{lh} \end{vmatrix}\psi = E\psi$$

where ψ is a 1 x 2 vector.

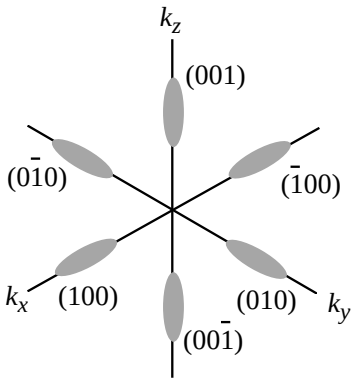
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BANDSTRUCTURE: SILICON

Although the bandstructure of Si is far from ideal, having an indicrect bandgap, hig hhole masses, and small spin-orbit splitting, processing related advantages make Si the premier semiconductor for consumer electronics. On the right we show constant energy ellipsoids for Si conduction band. There are six equivalent valleys in Si at the bandedge.



(a)



Six equivalent valleys at conduction bandedge

$$E_g = 1.17 - \frac{4.37 \times 10^{-4}\, T^2}{T - 636}\ (\text{eV}) \qquad T = \text{Temperature in K}$$

(b)

• Indirect gap material $\Rightarrow$ weak optical transitions, cannot be used to produce lasers.

• Valleys along the x-axis and $-x$-axis: $k_{0x} = \frac{2\pi}{a}$ (0.85,0,0) and $k_{0x} = \frac{2\pi}{a}$ (–0.85,0,0):

$$E(k) = E_c + \frac{\hbar^2}{2}\left[\frac{(k_x - k_{0x})^2}{m_l^*} + \frac{k_y^2 + k_z^2}{m_t^*}\right];\ m_l = 0.98\ m_0;\ m_t = 0.19\ m_0$$

similar E-k relations for other 4 valleys.

• Density of states mass = 1.08 m_0 (6 valleys included).

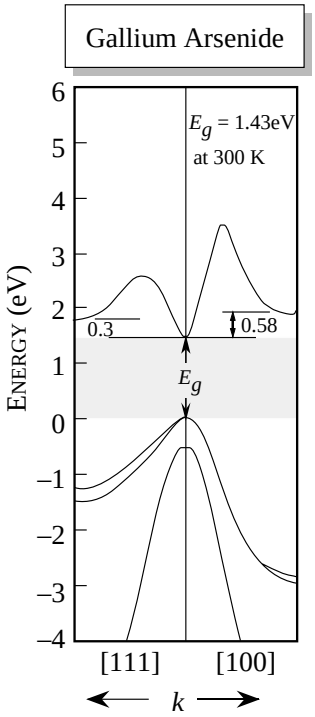
• Heavy hole mass: 0.49 m_0 ; light hole mass: 0.16 m_0.

• Intrinsic carrier concentration at 300 K: 1.5×10^{10} cm^{-3}.

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BANDSTRUCTURE: GaAs

The bandgap at 0 K is 1.51 eV and at 300 K it is 1.43 eV. The bottom of the conductionband is at k = (0,0,0), i.e., the G-point. The upper conduction band valleys are at the L-point.



$$E_g = 1.519 - \frac{5.4 \times 10^{-4}\, T^2}{T + 204} \text{ (eV)}$$

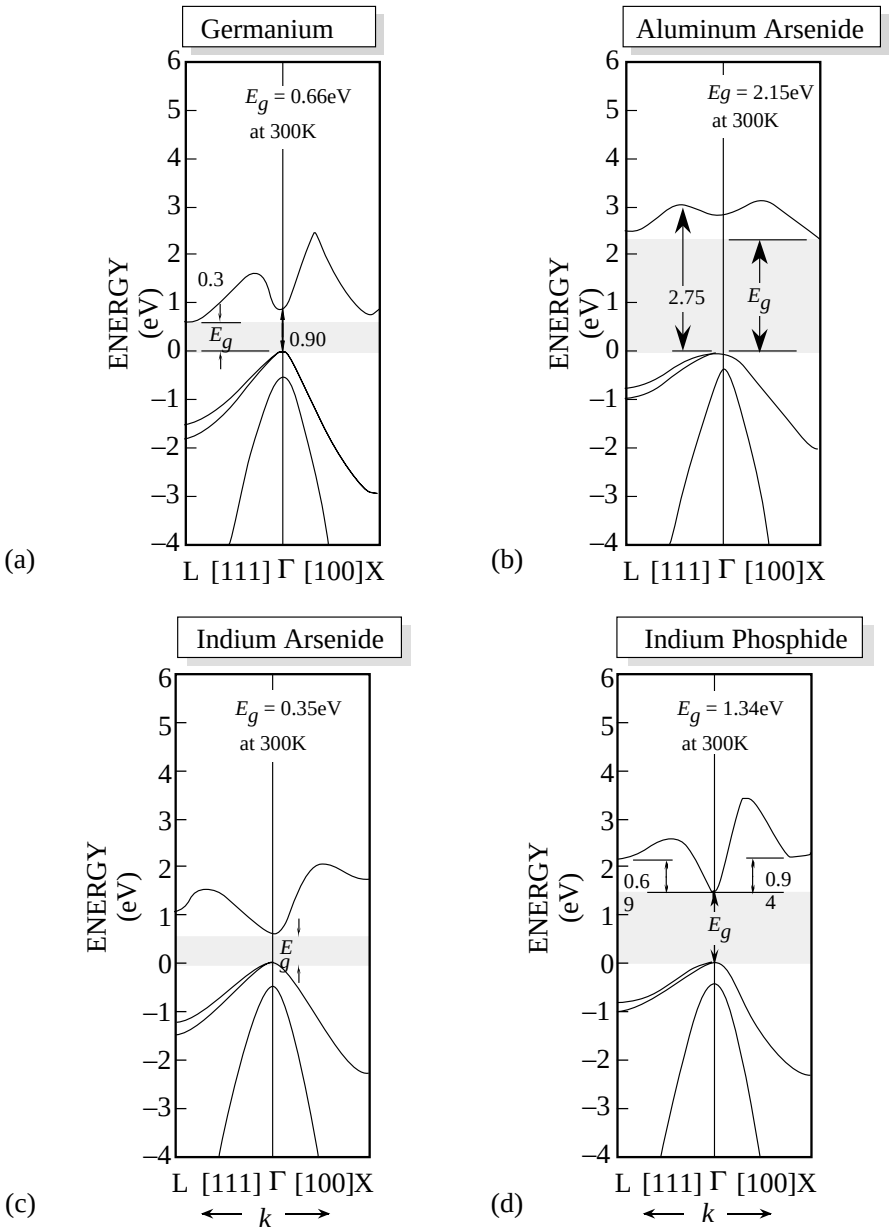
T = Temperature in K

CONDUCTION BAND: • Electron mass is light. $m^* = 0.067\, m_0$
• Upper valley mass is large. $m^* = 0.25\, m_0$ results in negative differential resistance at higher fields.
• Material is direct bandgap and has strong optical transistions $\Rightarrow$ can be used for light emission.

VALENCE BAND: • Heavy hole mass: 0.45 m_0; light hole mass = 0.08 m_0.
Intrinsic carrier concentration at 300 = 1.84×10^6 cm^{-3}.

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BANDSTRUCTURE: Ge AlAs, InAs, InP



(a) Bandstructure of Ge. (b) Bandstructure of AlAs. (c) Bandstructure of InAs. Since no adequate substitute matches InAs directly, it is often used as an alloy (InGaAs, InAlAs, etc.,) for devices. (d) Bandstructure of InP. InP is a very important material for high speed devices as well as a substrate and barrier layer material for semiconductor lasers.

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ELECTRONIC PROPERTIES OF SOME SEMICONDUCTORS

Material	Bandgap (eV)	Relative Dielectric Constant
C	5.5, I	5.57
Si	1.124, I	11.9
Ge	0.664, I	16.2
SiC	2.416, I	9.72
GaAs	1.424, D	13.18
AlAs	2.153, I	10.06
InAs	0.354, D	15.15
GaP	2.272, I	11.11
InP	1.344, D	12.56
InSb	0.230, D	16.8
CdTe	1.475, D	10.2
AlN	6.2, D	9.14
GaN	3.44, D	10.0
ZnSe	2.822, D	9.1
ZnTe	2.394, D	8.7

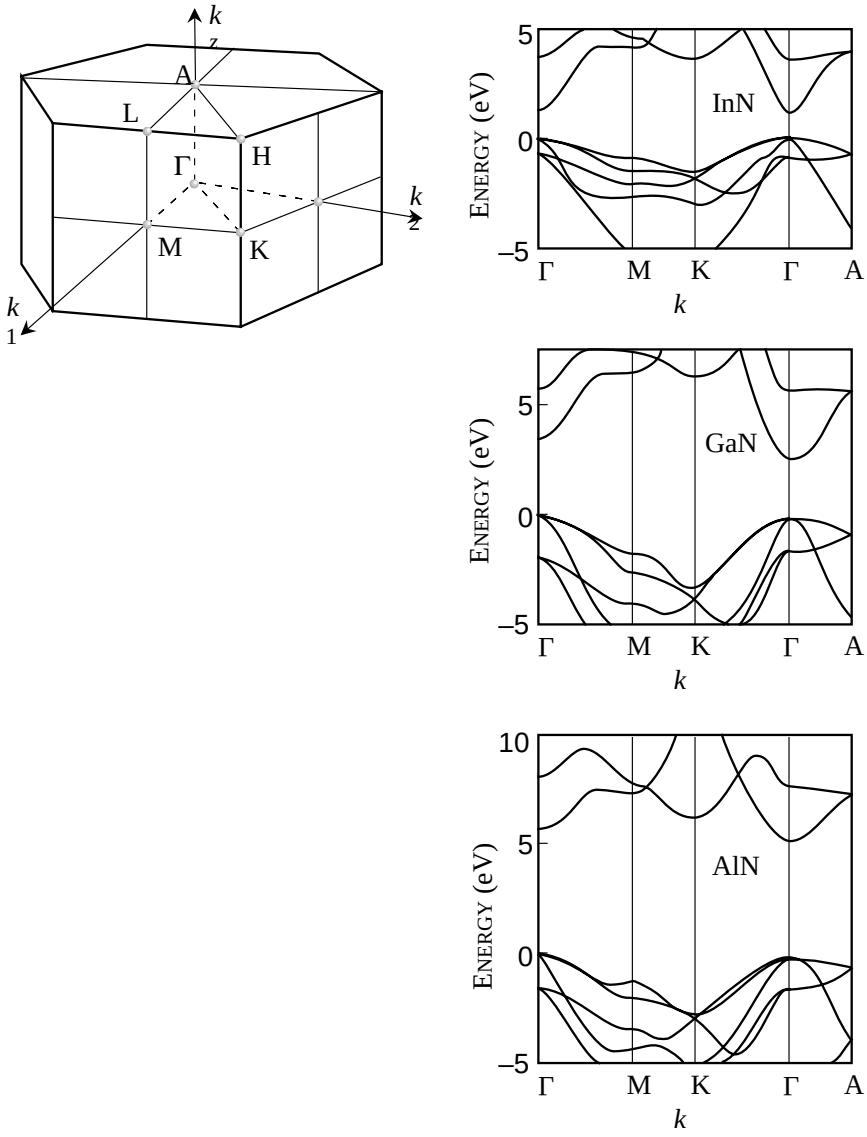
Material	Electron Mass (m_0)	Hole Mass (m_0)
AlAs	0.1	
AlSb	0.12	$m^*_{dos} = 0.98$
GaN	0.19	$m^*_{dos} = 0.60$
GaP	0.82	$m^*_{dos} = 0.60$
GaAs	0.067	$m^*_{lh} = 0.082$ $m^*_{hh} = 0.45$
GaSb	0.042	$m^*_{dos} = 0.40$
Ge	$m_l = 1.64$ $m_t = 0.082$ $m_{dos} = 0.56$	$m^*_{lh} = 0.044$ $m^*_{hh} = 0.28$
InP	0.073	$m^*_{dos} = 0.64$
InAs	0.027	$m^*_{dos} = 0.4$
InSb	0.13	$m^*_{dos} = 0.4$
Si	$m_l = 0.98$ $m_t = 0.19$ $m_{dos} = 1.08$	$m^*_{lh} = 0.16$ $m^*_{hh} = 0.49$

Properties of some semiconductors. D and I stand for direct and indirect gap, respectively. The data are at 300 K. Note that Si has six conducton band valleys, while Ge has four.

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BANDSTRUCTURE OF InN, GaN, AlN

These materials are important for blue light emission and high power/high temperature electronics.



Bandstructure of InN, GaN, and AlN. Also shown is the Brillioun zone.

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SOME IMPORTANT PROPERTIES OF Si AND GaAs

PROPERTY	SI	GAAS
Electron effective mass (m_0)	$m^*_l = 0.98$ $m^*_t = 0.19$ $m^*_{dos} = 1.08$ $m^*_\sigma = 0.26$	$m^* = 0.067$
Hole effective mass (m_0)	$m^*_{hh} = 0.49$ $m^*_{lh} = 0.16$ $m^*_{dos} = 0.55$	$m^*_{hh} = 0.45$ $m^*_{lh} = 0.08$ $m^*_{dos} = 0.47$
Bandgap (eV)	$1.17 - \frac{4.37 \times 10^{-4} T^2}{T + 636}$	$1.519 - \frac{5.4 \times 10^{-4} T^2}{T + 204}$
Electron affinity (eV)	4.01	4.07

For Si: m^*_{dos}: To be used in calculating density of states, position of Fermi level
m^*_σ: To be used in calculating response to electric field, e.g., in mobility

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HOLES IN SEMICONDUCTORS: WHAT ARE HOLES?

In a filled band (valence band) no current can flow, since electrons are normally Fermi particles and obey the Pauli exclusion principle. The electrons can "move" if there is an empty state available. The empty states in the valence band are called holes.

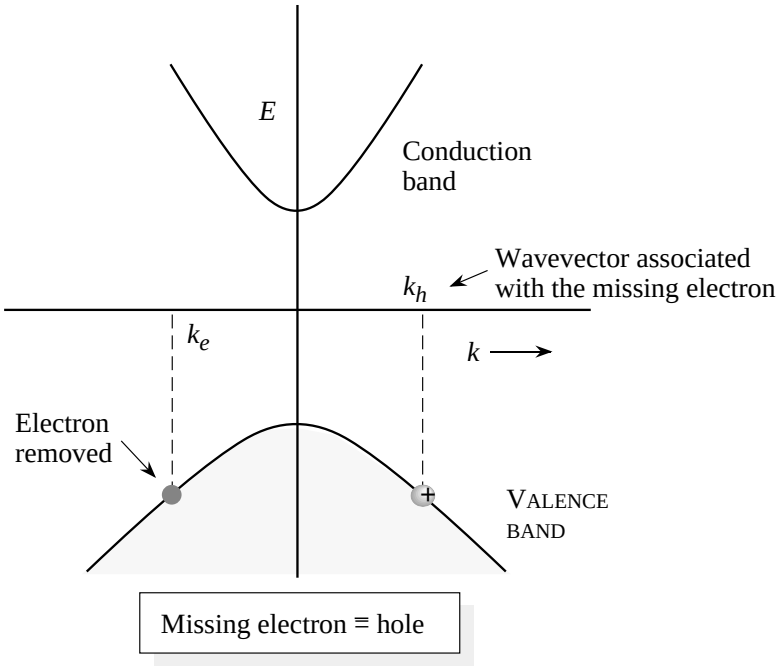


Diagram illustrating the wavevector of the missing electron k_e. The wavevector of the system with the missing electron is $-k_e$, which is associated with the hole.

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