

SEMICONDUCTOR PHYSICS REVIEW – BONDS, BANDS, EFFECTIVE MASS, DRIFT, DIFFUSION, GENERATION, RECOMBINATION

February 3, 2011

The University of Toledo, Department of Physics and Astronomy
SSARE, PVIC

Principles and Varieties of Solar Energy (PHYS 4400)
and
Fundamentals of Solar Cells (PHYS 6980)

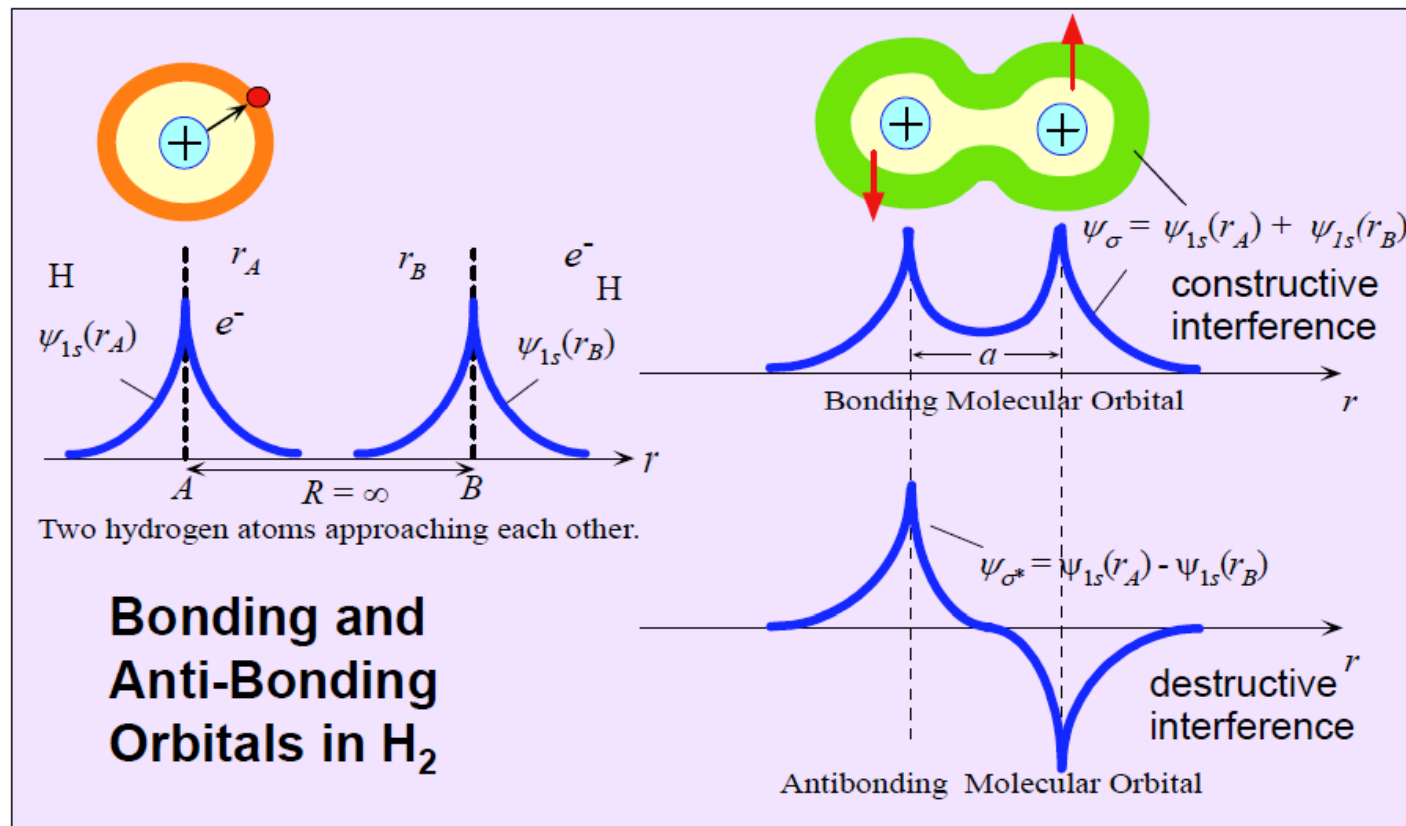


On today's menu

- Review of semiconductor physics
 - bonds and bands in crystals
 - electrons and holes
 - valence/conduction bands,
 - HOMO-LUMO concepts
- drift and diffusion
- photogenerated carriers
 - Absorption coefficient, depth dependence
 - direct vs. indirect gap
- recombination mechanisms

Quiz #2 next Tuesday, Feb. 8th





Formation of molecular orbitals, bonding and antibonding (ψ_σ and ψ_{σ^*}) when two H atoms approach each other. The two electrons pair their spins and occupy the bonding orbital ψ_σ .

5Fig 4.1

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Molecular Orbitals of H₂

In bringing the two atoms together, the two identical 1s atomic orbitals indicated by the wavefunctions $\psi_{1s}(\mathbf{r})$, that can accommodate two electrons each in the two isolated atoms, evolve into two molecular orbitals that can do the same in the molecule, but without violation of the Pauli Exclusion Principle.

Thus, as the two atomic orbitals interact, they lead to two new one electron wavefunctions with different energy levels and accommodating two electrons each, with four different sets of quantum numbers, i.e., four states in all.

The interaction can lead to constructive or destructive interference of the one electron wavefunctions:

$$\psi_{\sigma}^{(g)} = \frac{\psi_{1s}(\mathbf{r}_A) + \psi_{1s}(\mathbf{r}_B)}{[2(I + 1)]} \quad \psi_{\sigma^*}^{(u)} = \frac{\psi_{1s}(\mathbf{r}_A) - \psi_{1s}(\mathbf{r}_B)}{[2(I + 1)]}$$

I is an "overlap integral" used for normalization. This approach to generating molecular orbitals is the LCAO method described on the previous slide.

The + sign corresponds to a molecular orbital that is spatially symmetric with respect to the midpoint between the atoms (labeled "g" for *gerade* or *even*) and

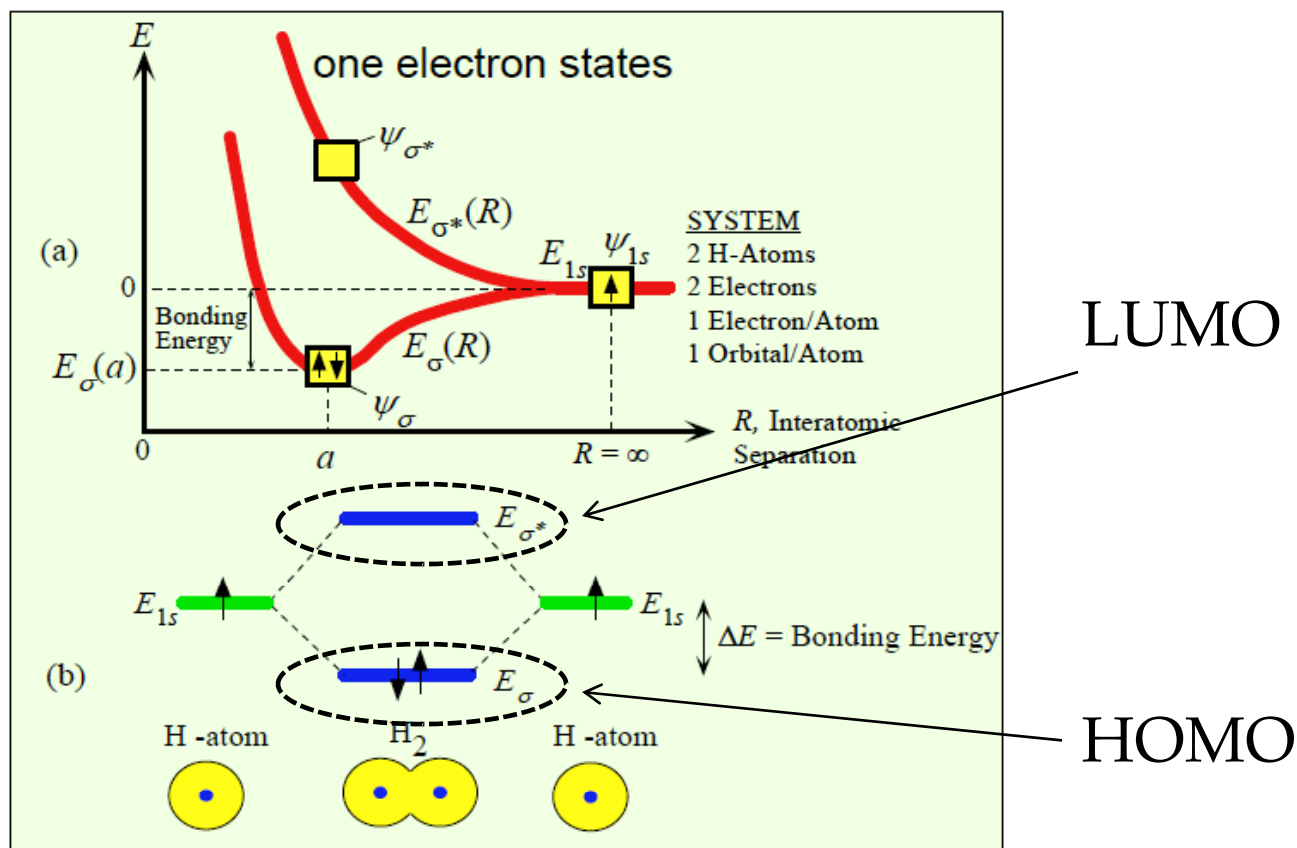
the – sign corresponds to a spatially antisymmetric orbital ("u" for *ungerade* or *odd*).

For the + sign, the electron density between the two protons is higher; this effect leads to a lower potential energy by enabling the electron density to be close to two protons simultaneously, a characteristic of a *bonding orbital*.

For the – sign, a node in the electron density exists between the atoms; this configuration leads to a higher energy level, a characteristic of an *antibonding orbital*.



Electronic Energy Levels of the H₂ Molecule



Electron energy in the system comprising two hydrogen atoms. (a) Energy of ψ_σ and ψ_{σ^*} vs. the interatomic separation, R . (b) Schematic diagram showing the changes in the electron energy as two isolated H atoms, far left and far right, come together to form a hydrogen molecule.

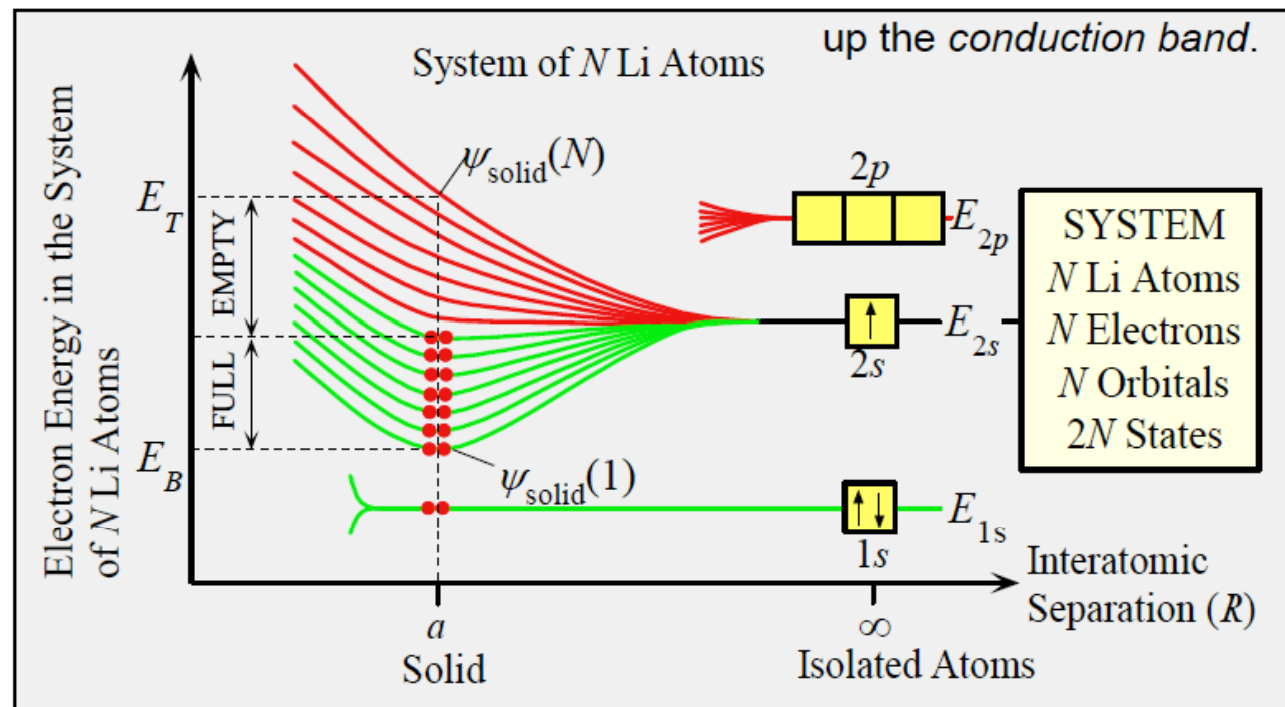
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Band Theory of Solids

The full 1s atomic states form full 1s core states in the solid.

The half-filled 2s atom states form half-filled 2s valence states in the solid that make up the *conduction band*.

N "levels"
 $2N$ "states"

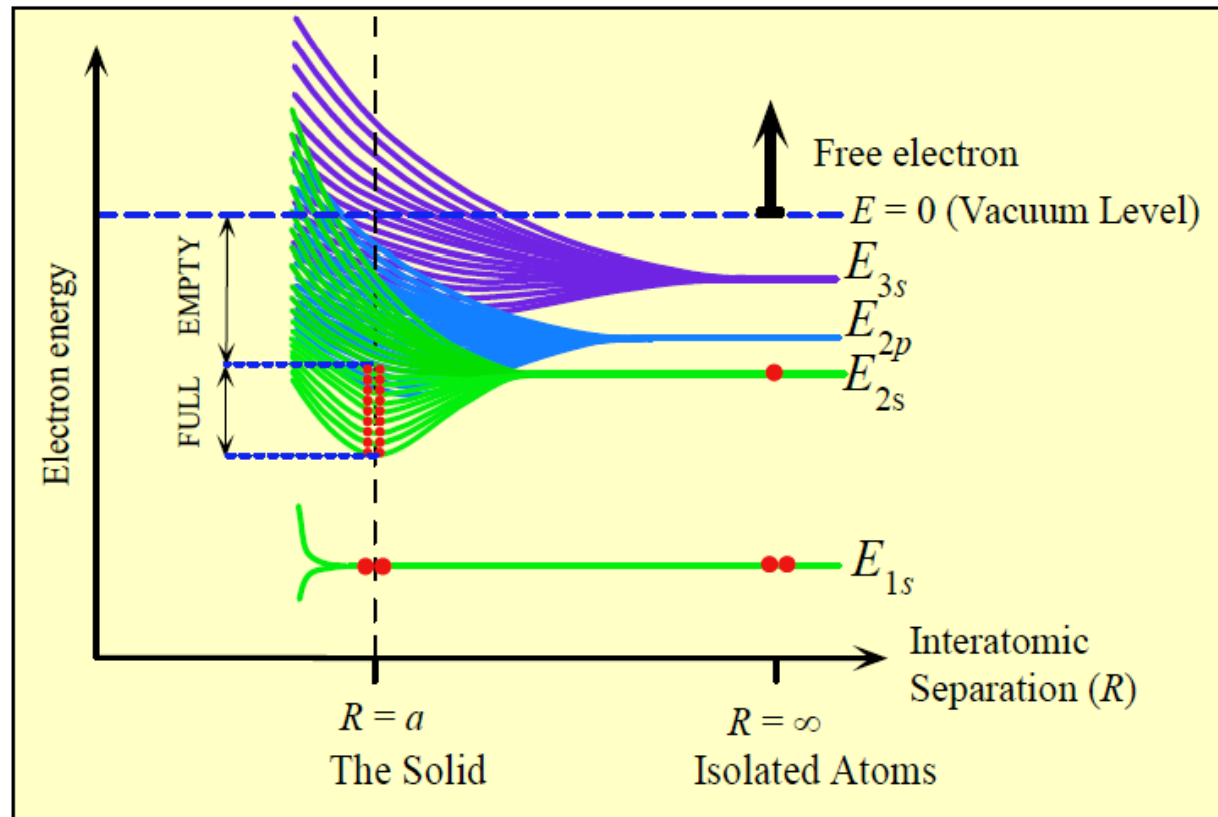


The formation of a $2s$ -energy band from the $2s$ -orbitals when N Li atoms come together to form the Li solid. There are N $2s$ -electrons but $2N$ states in the band. The $2s$ -band therefore is only half full. The atomic $1s$ orbital is close to the Li nucleus and remains undisturbed in the solid. Thus each Li atom has a closed K -shell (full $1s$ orbital).

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Band Theory of Solids



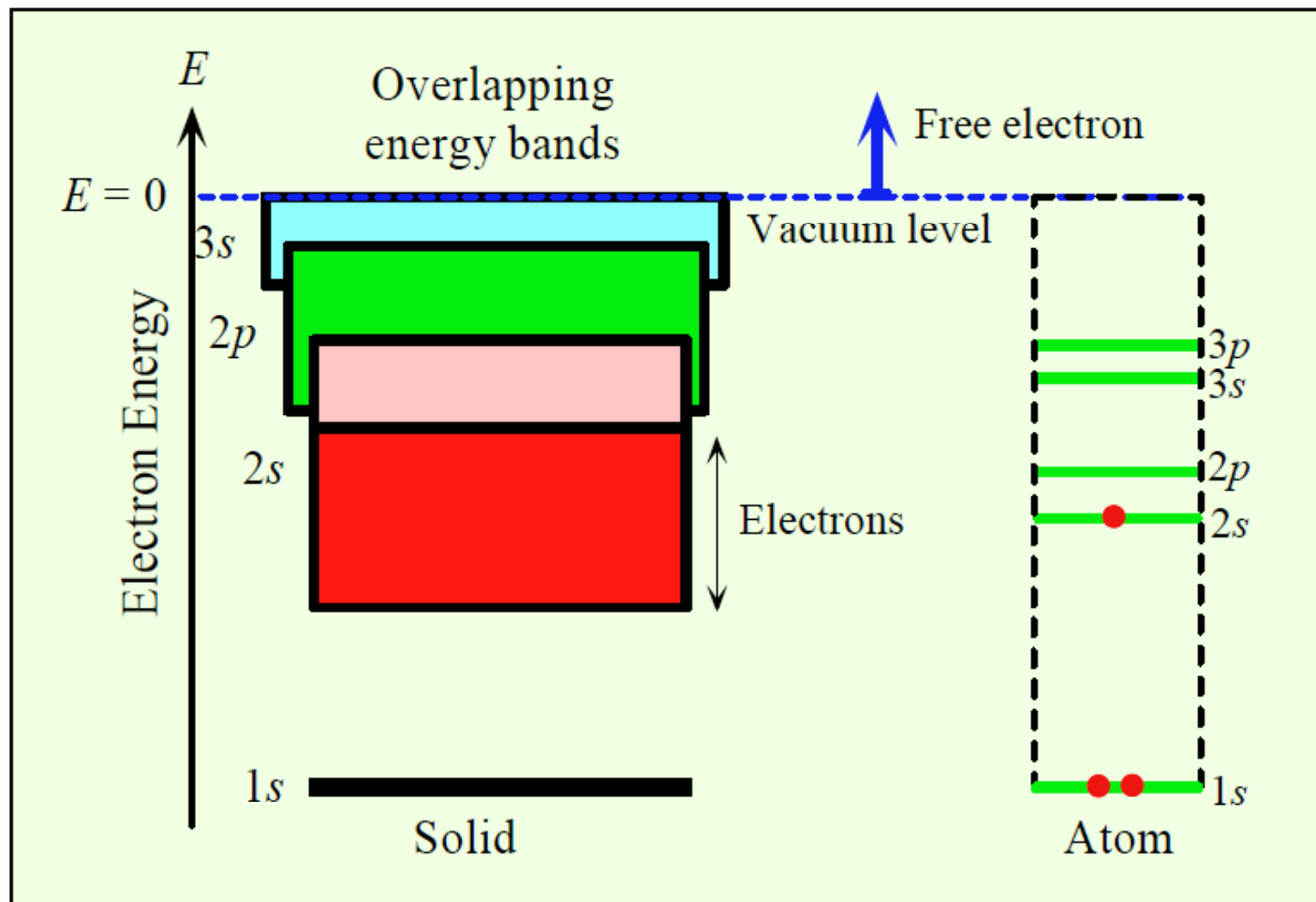
As solid atoms are brought together from infinity, the atomic orbitals overlap and give rise to bands. Outer orbitals overlap first. The $3s$ orbitals give rise to the $3s$ band, $2p$ orbitals to the $2p$ band and so on. The various bands overlap to produce a single band in which the energy is nearly continuous.

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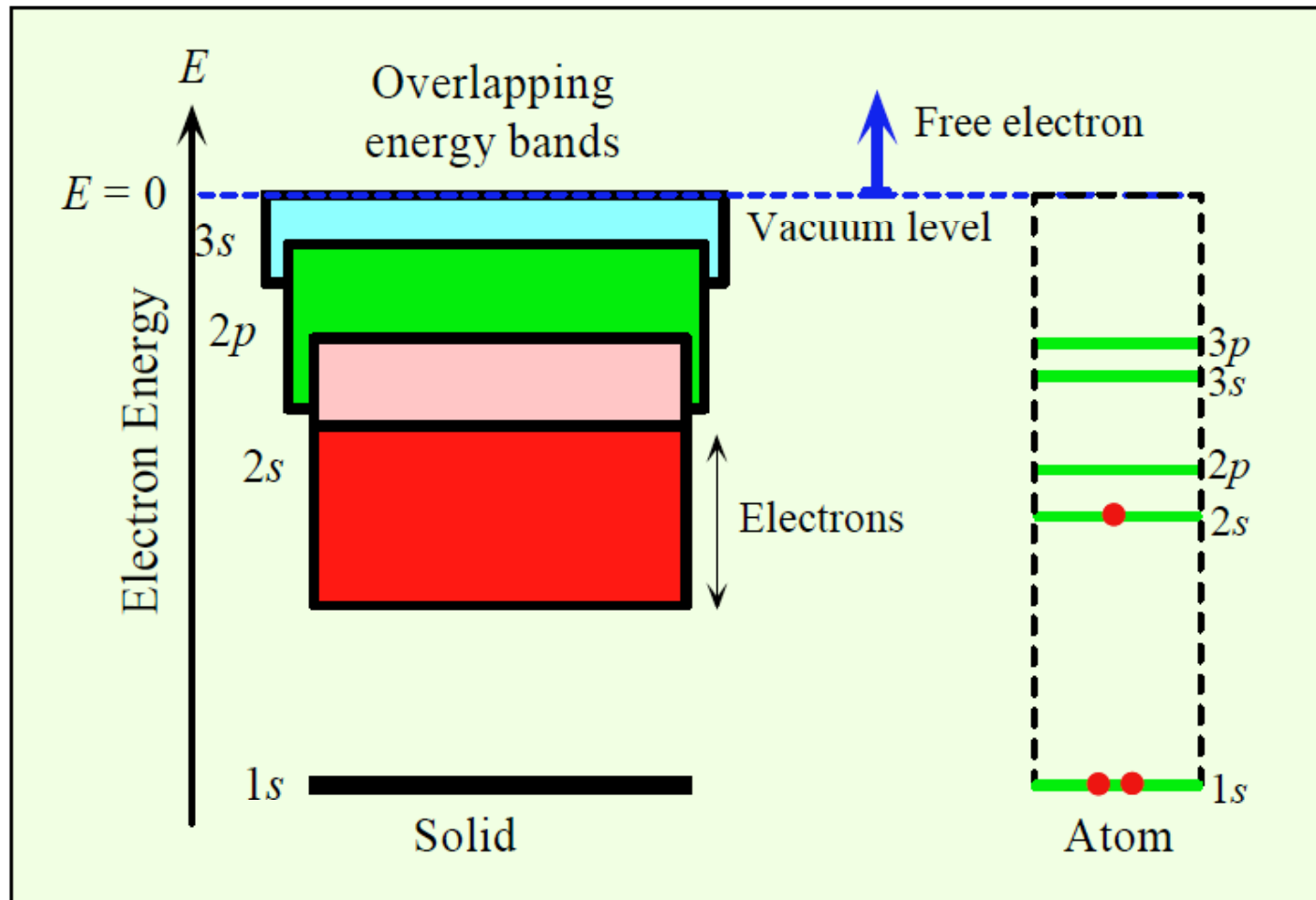
Band Theory of Solids



In a metal the various energy bands overlap to give a single band of energies that is only partially full of electrons. There are levels with energies up to the vacuum level where the electron is free.

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Band Theory of Solids



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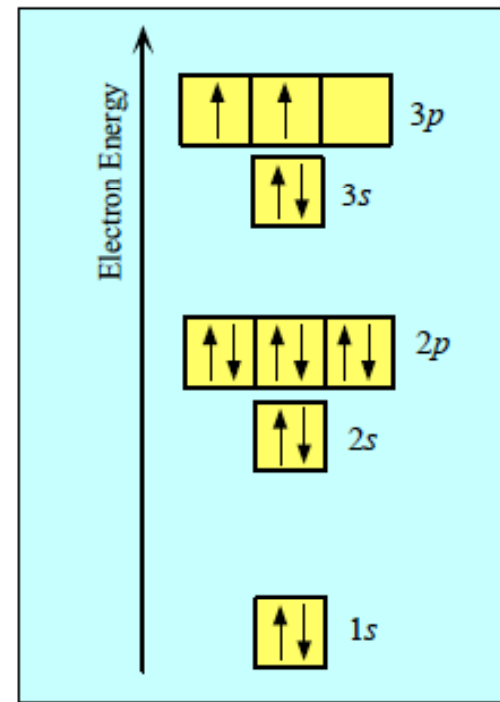
Semiconductors

As a prototypical semiconductor, consider Si which has 14 electrons.

When atoms are brought together to form a solid, the filled $n = 1$ and $n = 2$ shells act as core electrons and do not participate in the bonding. Thus, they show little energy spread in the solid.

The 4 valence electrons with $n = 3$ have energies that are relatively close. So when five Si atoms are brought together, the orbitals that interact are the $3p$ and $3s$. What is found is that the orbitals reorganize to maximize the overlap in three dimensions in a process called *hybridization*.

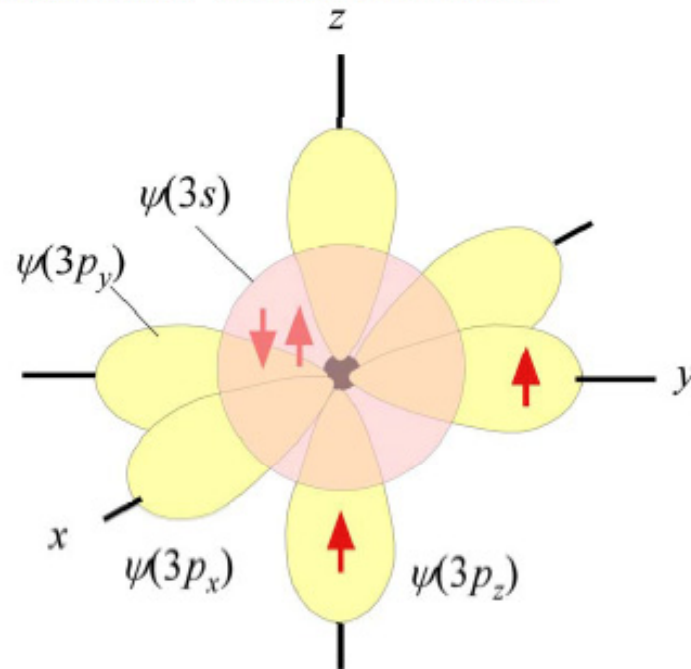
The valence electrons of atoms considered so far have been in partially filled s states ($l = 0$) which are non-directional and so do not show such an effect. As a result, an atom such as Li forms a BCC crystal and one electron per Li atom is free to move throughout the crystal.



The four atomic orbitals $\psi(3s)$, $\psi(3p_x)$, $\psi(3p_y)$, $\psi(3p_z)$ with a capacity of 8 electrons hybridize into four sp^3 molecular orbitals oriented in a tetrahedron also with a capacity of 8 electrons (see next slide).

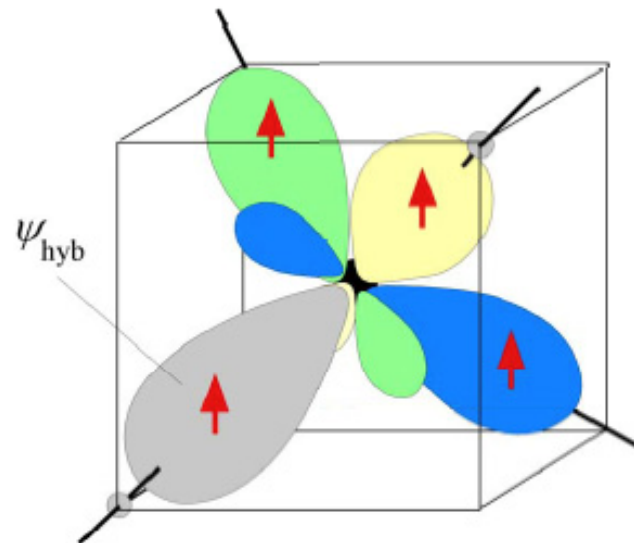


Isolated Silicon Atom



(a) Isolated Si

Silicon Atom in a Solid



(b) Si before it bonds

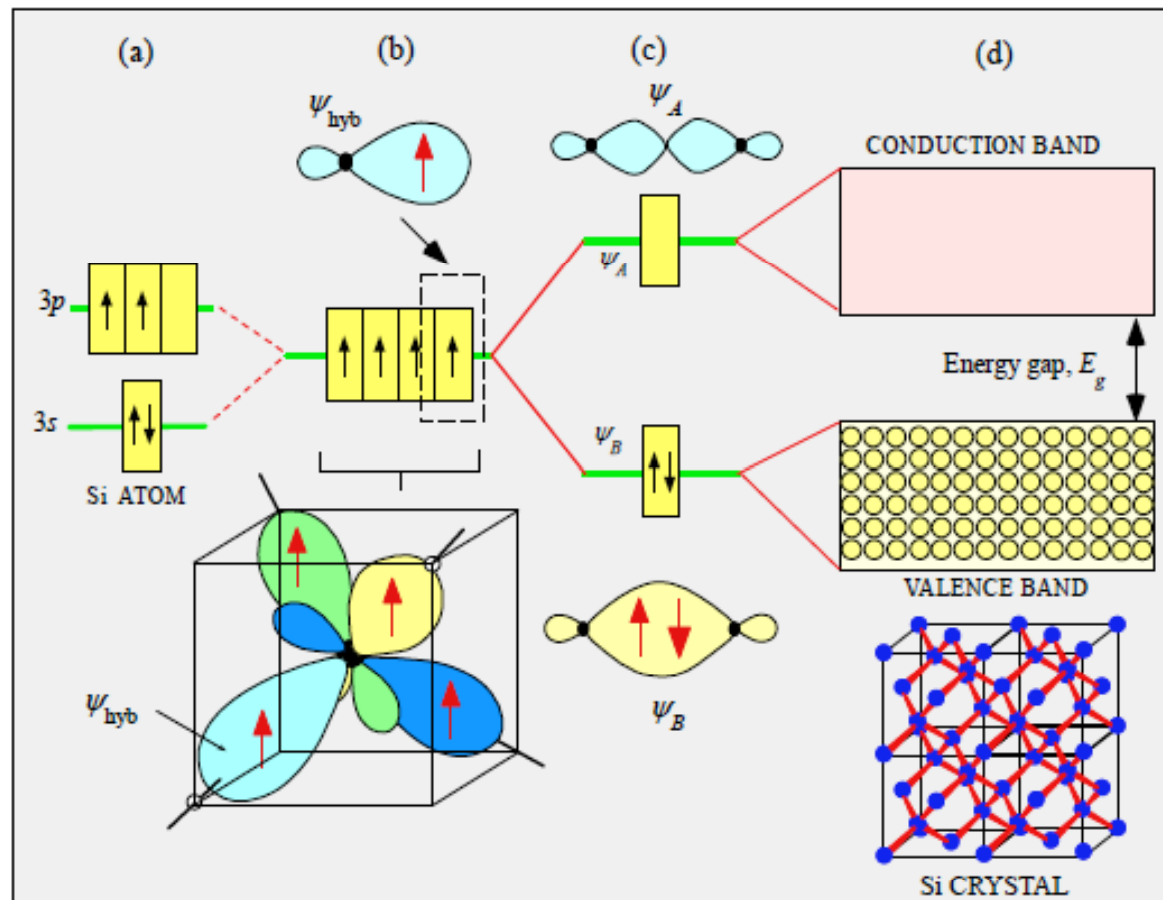
Molecular Orbitals from Hybridization of Atomic Orbitals

(a). Si is in Group IV in the Periodic Table. An isolated Si atom has 2 electrons in the 3s and 2 electrons in the 3p orbitals. (b) When Si is about to bond, the *one* 3s-orbital and the *three* 3p-orbitals become perturbed and mixed to form four hybridized orbitals, ψ_{hyb} , called sp^3 orbitals which are directed towards the corners of a tetrahedron. The ψ_{hyb} orbital has a large major lobe and a small back lobe. Each ψ_{hyb} orbital takes one of the four valence electrons.

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Formation of Energy Bands in Si by Splitting of Hybridized Molecular Orbitals

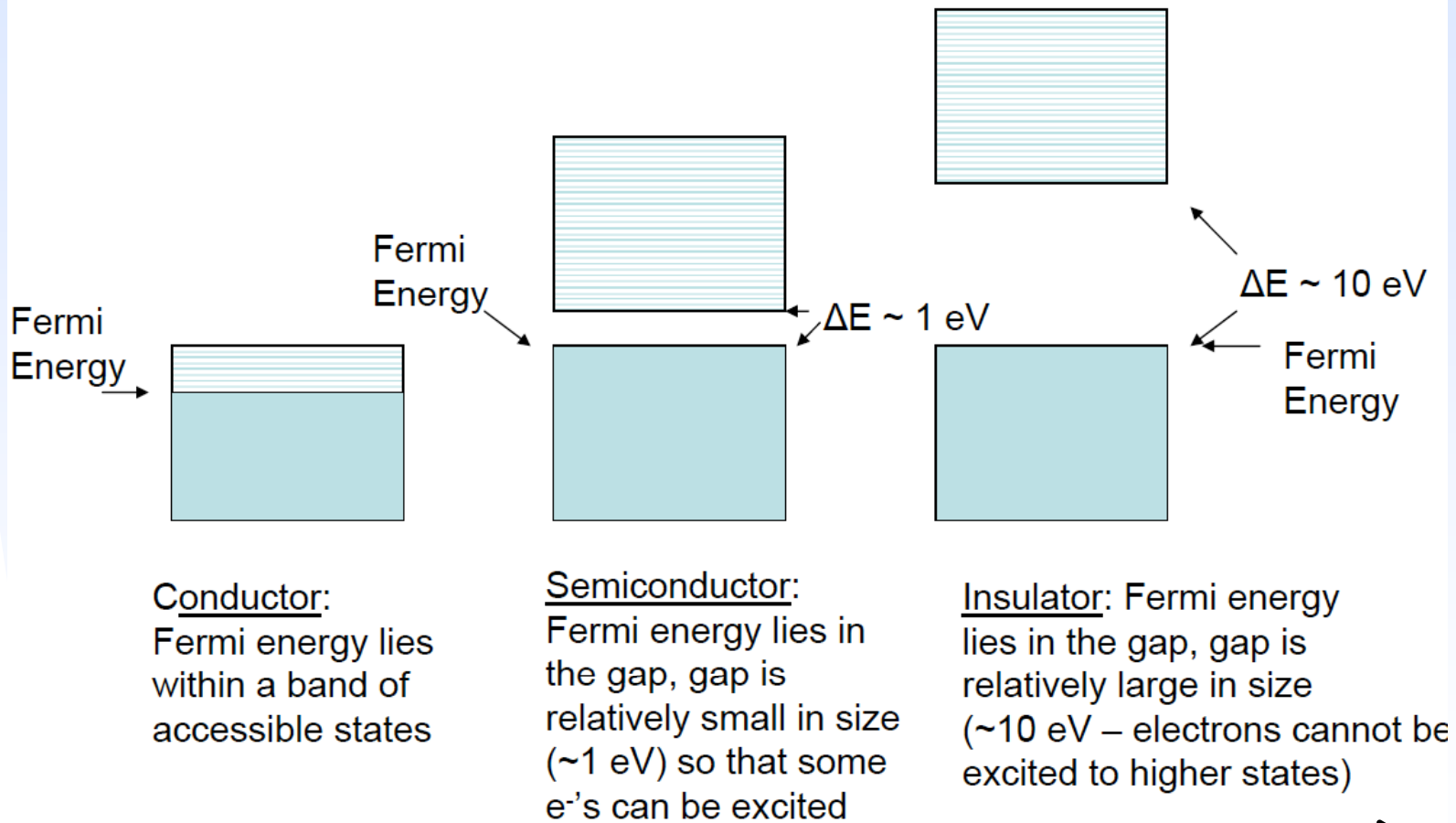


(a) Formation of energy bands in the Si crystal first involves hybridization of 3s and 3p orbitals to four identical ψ_{hyb} orbitals which make 109.5° with each other as shown in (b). (c) ψ_{hyb} orbitals on two neighboring Si atoms can overlap to form ψ_B or ψ_A . The first is a bonding orbital (full) and the second is an antibonding orbital (empty). In the crystal ψ_B overlap to give the valence band (full) and ψ_A overlap to give the conduction band (empty).

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Conductors, Insulators, Semiconductors



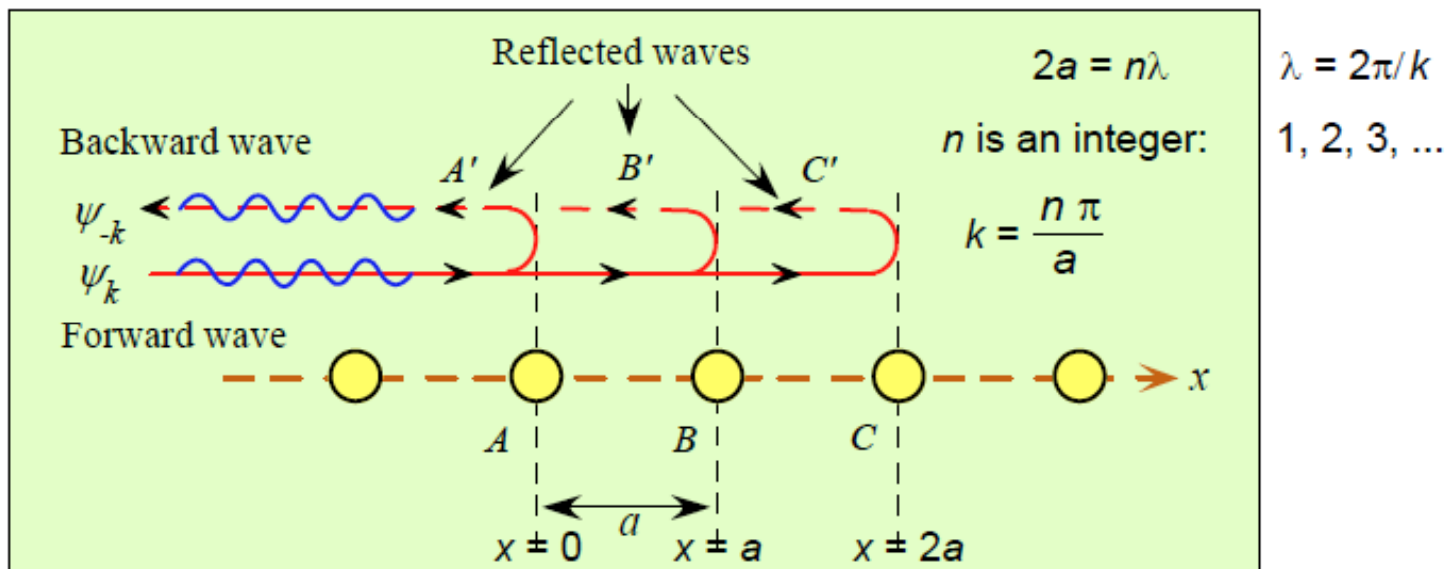
Charge carriers increasingly “feel” the crystal potential



Nearly-Free-Electron Model

Although we approximate $V(x) = 0$ within the crystal, the lattice sites generate periodic perturbations that lead to electron *diffraction* inside the crystal. This can happen in covalently bonded crystals also... the concept is not confined to metals.

Diffraction occurs with a reinforcing backward wave when the EPD or electron path difference, $2a$, is matched by an integral number of wavelengths $n\lambda$.



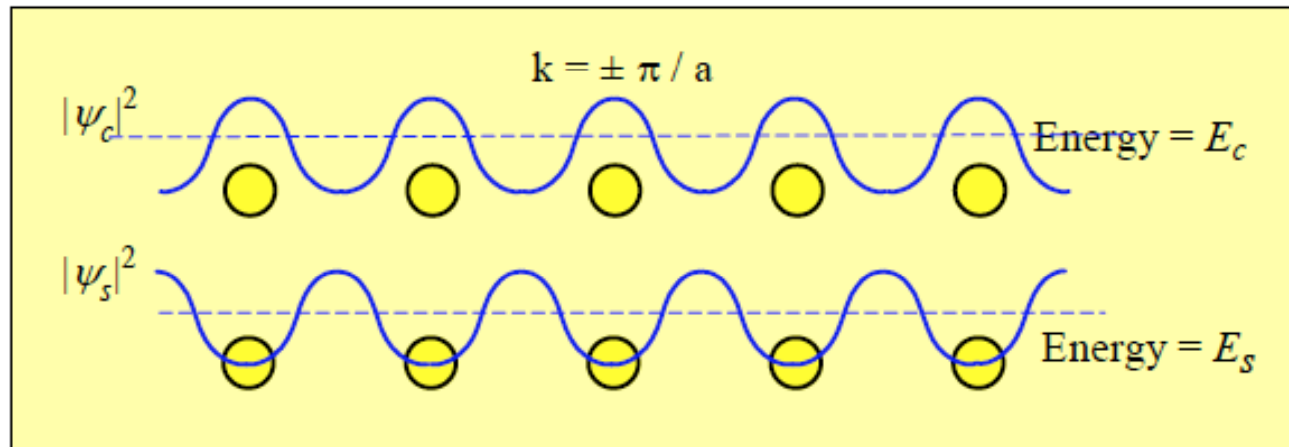
An electron wave propagation through a linear lattice. For certain k values the reflected waves at successive atomic planes reinforce each other to give rise to a reflected wave travelling in the backward direction. The electron then cannot propagate through the crystal.

At the Brillouin boundary



Nearly-Free-Electron Model

Given a single electron placed in a fixed periodic potential of positively charged atomic cores, the electron will achieve a lower energy configuration when it overlaps the cores most strongly. The potential energy will be negative in this case... call it $-V_n$. Now, $V_c + V_s$ is proportional to the average potential in the crystal, which for a weak potential vanishes. In addition, even if one adds the lowest order Fourier component to make the small potential periodic, then $V = V_0 \cos(2\pi x/a)$ and this also vanishes in the average.



Forward and backward waves in the crystal with $k = \pm \pi/a$ give rise to two possible standing waves, ψ_c and ψ_s . Their probability density distributions, $|\psi_c|^2$ and $|\psi_s|^2$, have maxima either at the ions or between the ions.



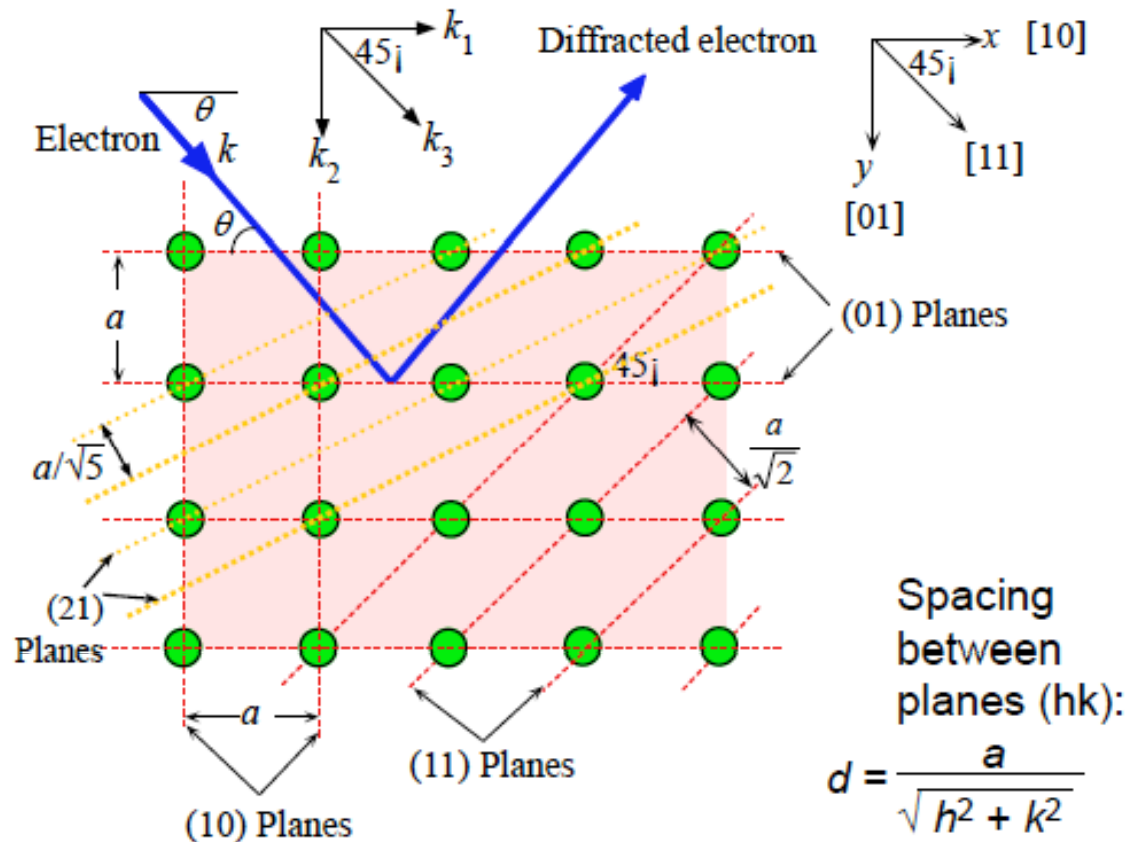
Nearly-Free-Electron Model

Consider the lowest band gap due to diffraction of electrons traveling in different directions:

For k along $[10]$, the first band gap occurs at $k = \pm \pi/a$ due to the (10) diffracting planes. For k along $[01]$ the behavior is the same.

For k along $[11]$, the first band gap occurs at $k = \pm \sqrt{2} (\pi/a)$ due to the $\{10\}$ diffracting planes with spacing a and $\theta=45^\circ$.

Diffraction also occurs for this same k due to the (11) planes with $\theta=0^\circ$ and spacing $a/\sqrt{2}$.



Diffraction of the electron in a two dimensional cubic crystal. Diffraction occurs whenever k has a component satisfying $k_1 = \pm n\pi/a$, $k_2 = \pm n\pi/a$ or $k_3 = \pm n\pi/a$. In general terms, when $k \sin \theta = n\pi/a$.



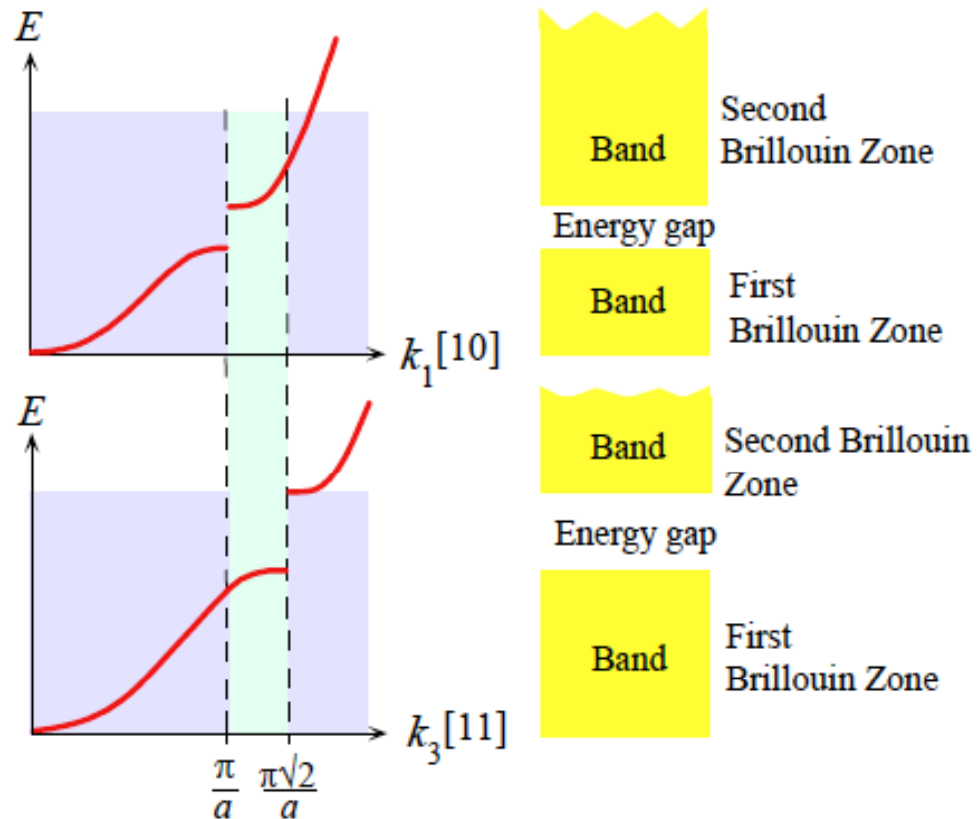
Nearly-Free-Electron Model

This figure shows that the position of the energy gap along a particular direction in k space and its magnitude depends on the direction.

The same general concept can be applied in three dimensions, as well.

Spacing between planes (hkl) in 3d in a cubic crystal:

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

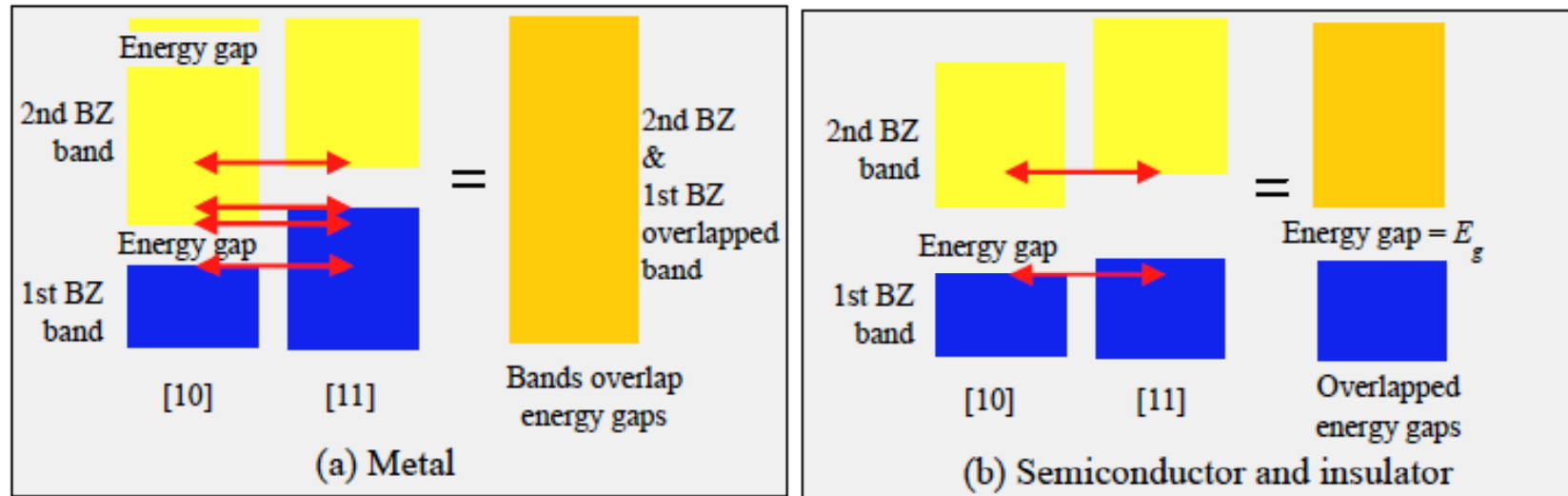


The E - k behavior for the electron along different directions in the two dimensional crystal. The energy gap along $[10]$ is at π/a whereas it is at $\pi\sqrt{2}/a$ along $[11]$.

14Fig 4.15

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Nearly-Free-Electron Model



(a) Metal: For the electron in a metal there is no apparent energy gap because the 2nd BZ (Brillouin Zone) along [10] overlaps the 1st BZ along [11]. Bands overlap the energy gaps. Thus the electron can always find an energy by changing its direction.

(b) Semiconductor or insulator: For the electron in a semiconductor there is an energy gap arising from the overlap of the energy gaps along [10] and [11] directions. The electron can never have an energy within this energy gap, E_g .

The red arrows show possible phonon scattering events which carry significant momentum and very little energy. Phonon scattering allows electrons in metals to increase and decrease continuously in energy without gaps simply by changing direction.

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Nearly-Free-Electron Model

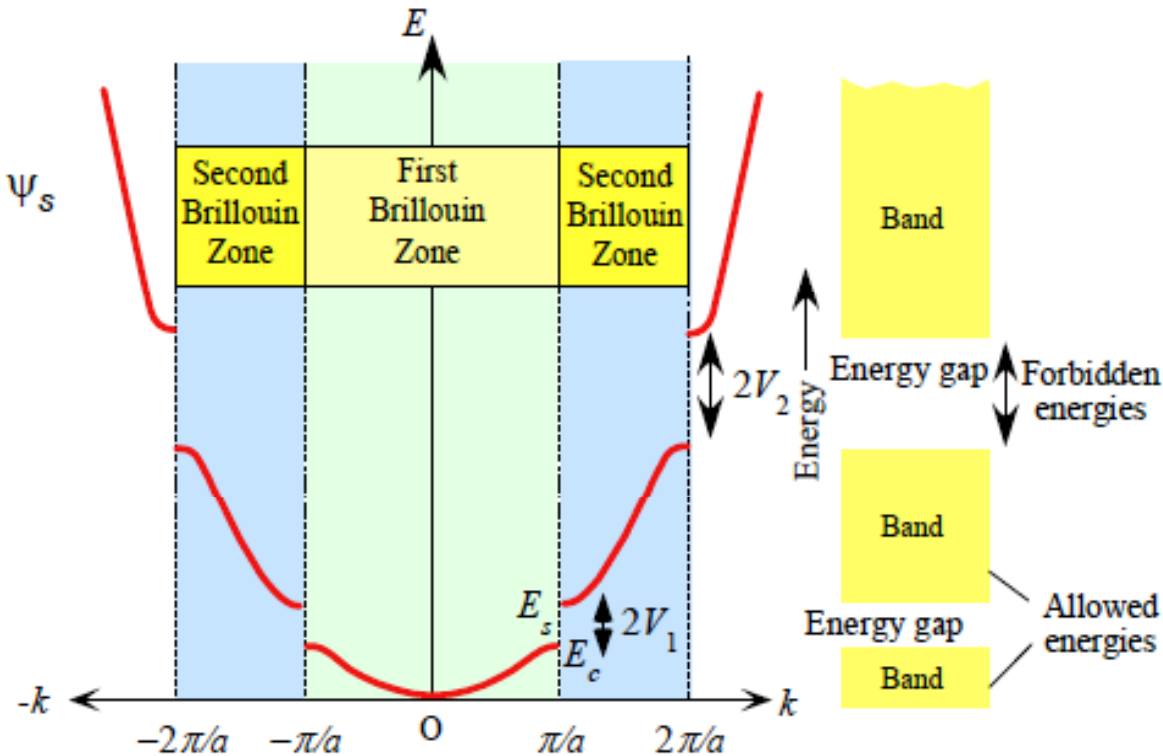
The total energy of the electrons having wavefunctions ψ_c and ψ_s are:

$$E_c \approx \frac{\hbar^2 k^2}{2m_e} - V_n$$

$$E_s \approx \frac{\hbar^2 k^2}{2m_e} + V_n$$

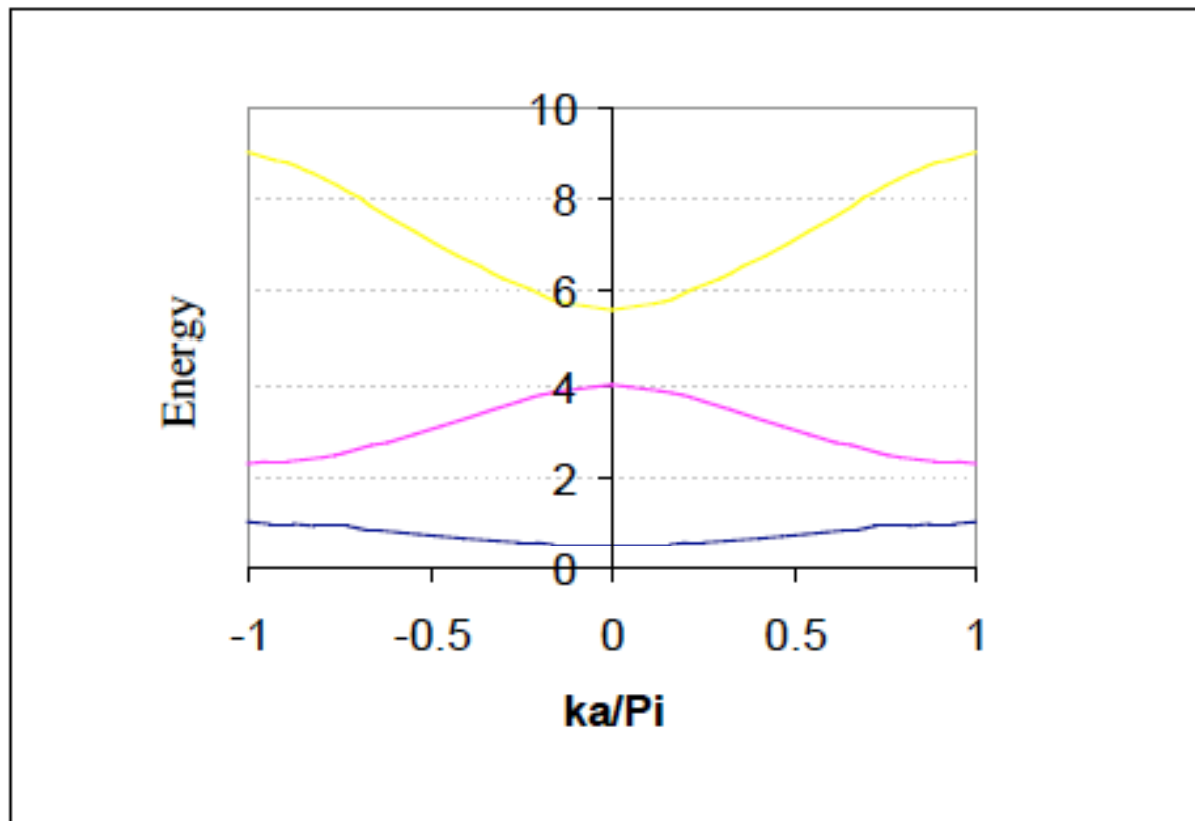
These wavefunctions have the same wave vector quantum number k but different energies by virtue of the different PE's.

For k values away from the Bragg reflection condition of $k=n\pi/a$, the waves continue to act as traveling waves.



The energy of the electron as a function of its wavevector k inside a one-dimensional crystal. There are discontinuities in the energy at $k = \pm n\pi/a$ values where the waves suffer Bragg reflections in the crystal. There are energy gaps at these k values. For example, there can be no energy value for the electron between E_c and E_s . $E_s - E_c$ is therefore an energy gap at $k = \pm\pi/a$. Away from the critical k values, the $E-k$ behavior is like that of a "free" electron, E increasing with k as $E = (\hbar k)^2/2m_e$. These energies fall within an energy band inside a solid.

Reduced Zone Scheme

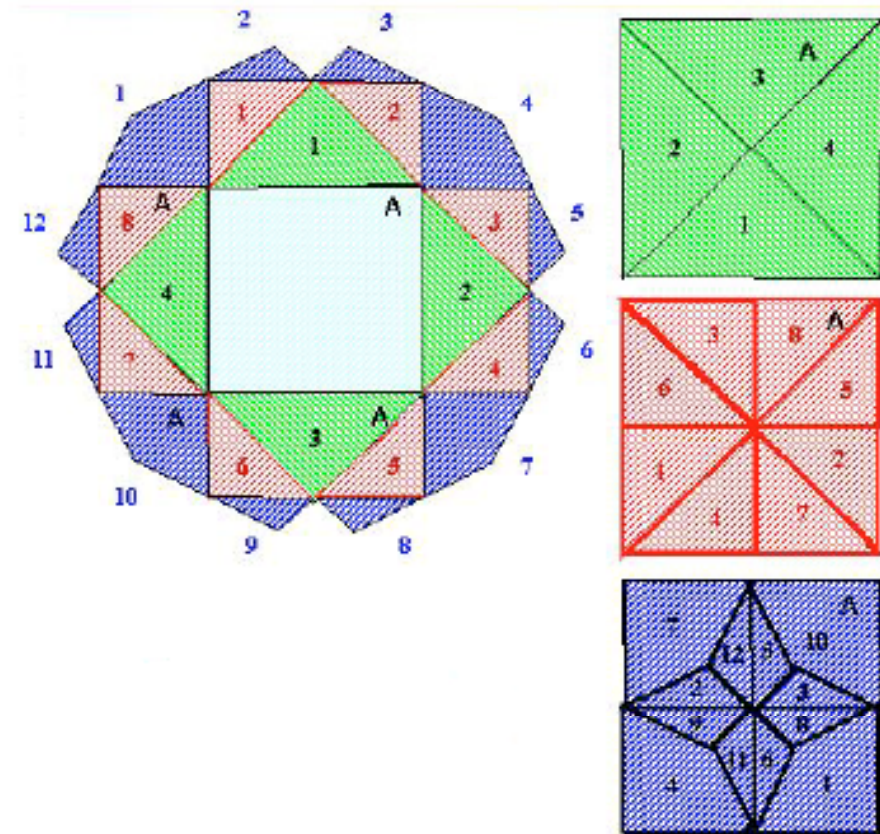


- Bands folded into First Brillouin Zone

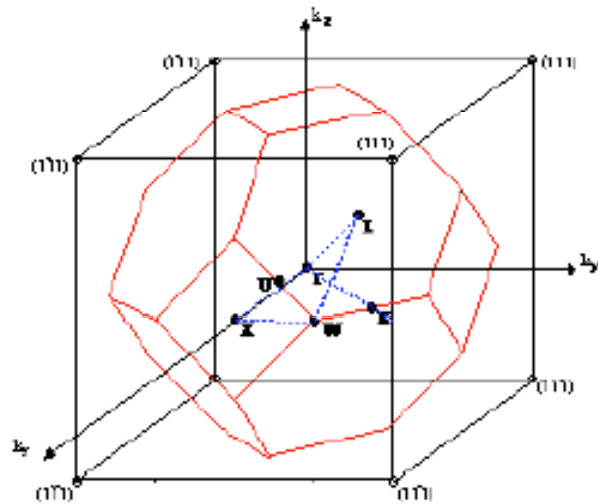


Brillouin zones -2D

- higher order zones can be mapped directly onto the 1st BZ by simple translation
- all BZs have exactly the same area/volume
- 1BZ corresponds to the primitive lattice cell in reciprocal space



Free electron bands for fcc structure



Γ – center of the BZ

X – [100] intercept;

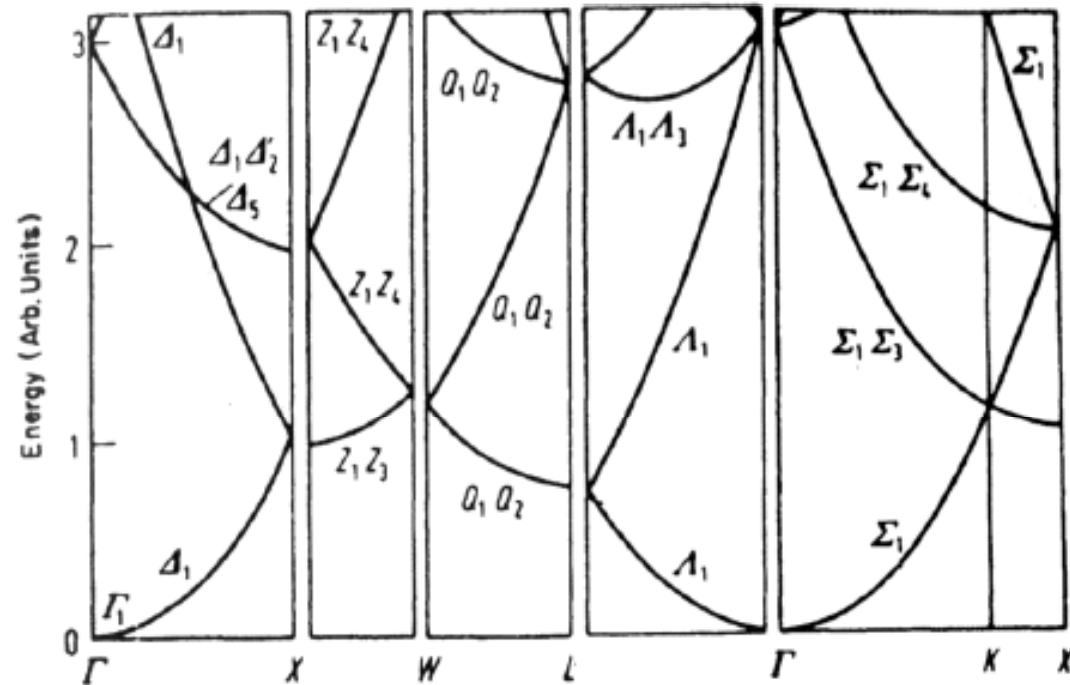
K – [110] intercept;

L – [111] intercept;

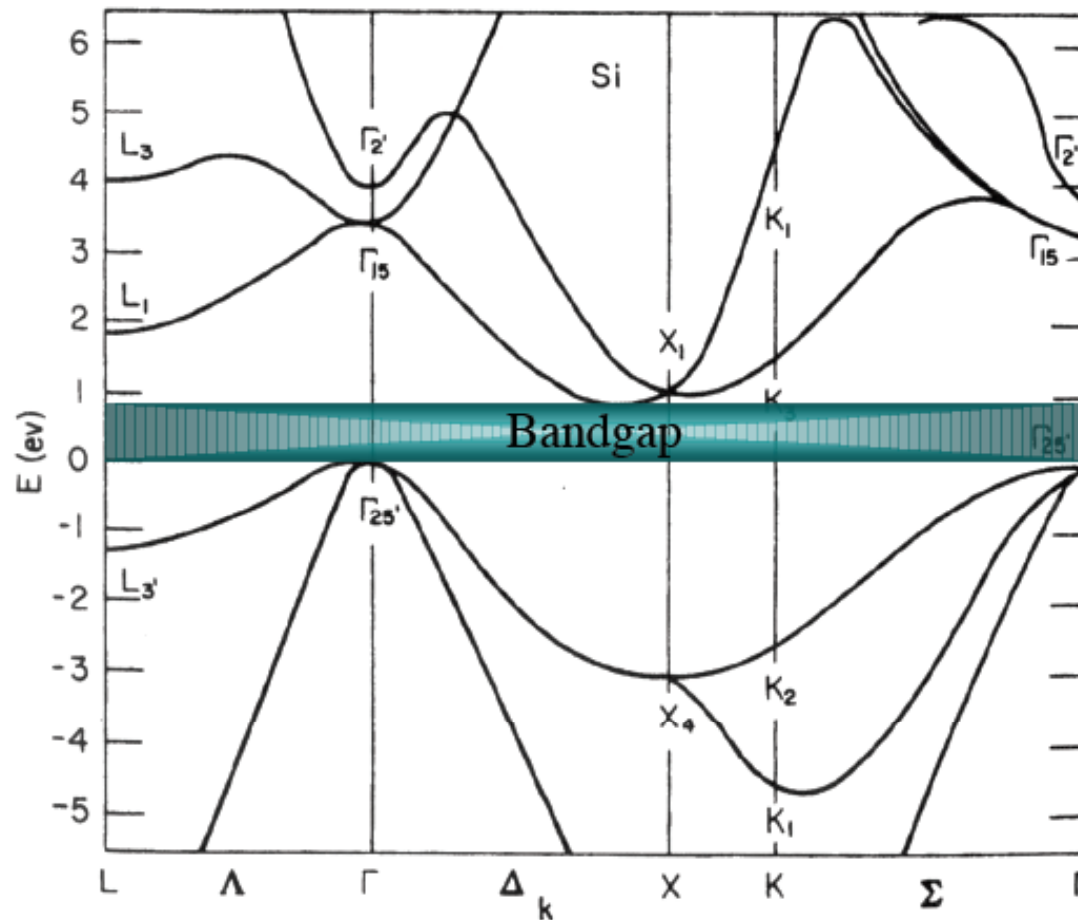
Γ – X path Δ

Γ – K path Σ

Γ – L path Λ



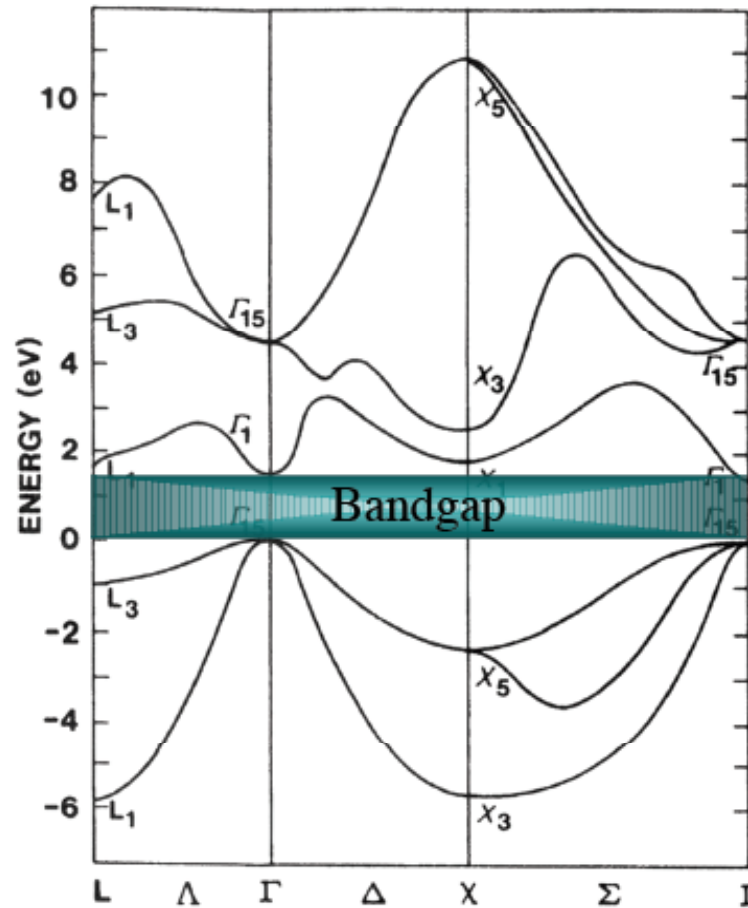
Band structure of Si (diamond)



Indirect Gap



Band structure of GaAs (zb)



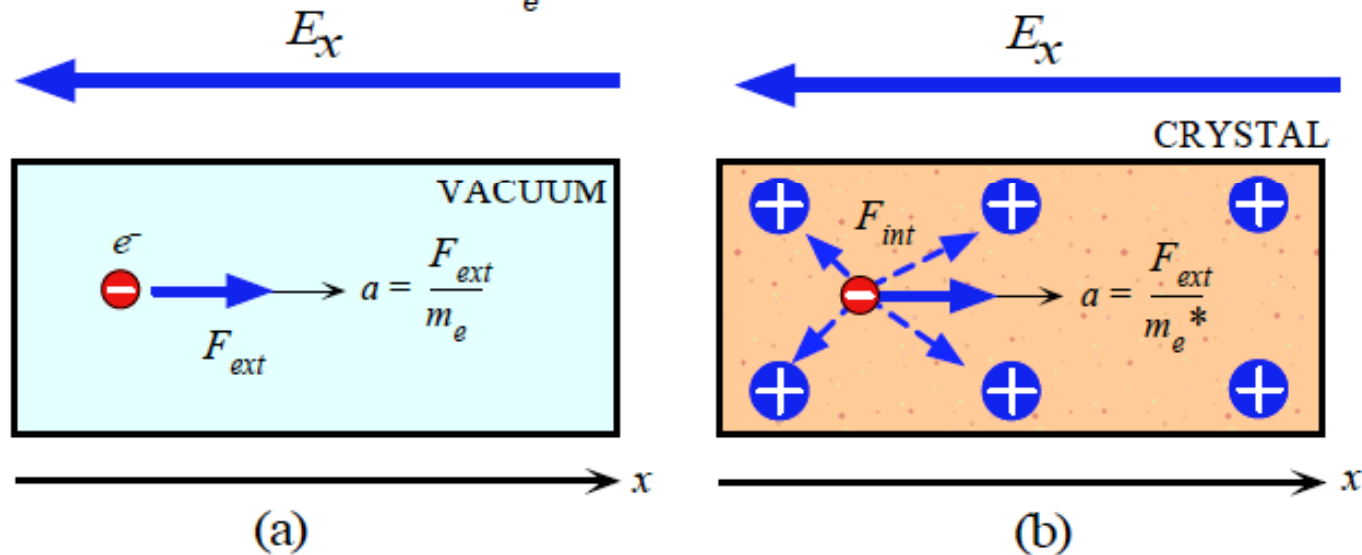
Direct Gap

Electron Effective Mass

The acceleration of an electron in a crystal a_c is influenced by both external and internal forces:

$$\mathbf{a}_c = (\mathbf{F}_{\text{ext}} + \mathbf{F}_{\text{int}})/m_e = (\mathbf{F}_{\text{ext}} - \vec{\nabla} V)/m_e \equiv \mathbf{F}_{\text{ext}}/m_e^*$$

When the band is not full, all the effects of both internal and external forces are incorporated into an effective mass m_e^* .



(a) An external force F_{ext} applied to an electron in vacuum results in an acceleration $a_{\text{vac}} = F_{\text{ext}} / m_e$. (b) An external force F_{ext} applied to an electron in a crystal results in an acceleration $a_{\text{cryst}} = F_{\text{ext}} / m_e^*$. (E_x is the electric field.)



Electron Effective Mass

One can apply the concept of the group velocity to a wavefunction defined as a traveling wave $\Psi(x, t) = A \exp\{i(k_x x - \omega t)\}$; $\omega = E_k/\hbar$ with wave vector k_x .

The group velocity is $v_{gx} = \frac{d\omega}{dk_x}$

$$\frac{dv_{gx}}{dt} = \frac{1}{\hbar} \frac{d^2 E_k}{dk_x^2} \frac{dk_x}{dt}$$

Note that:

$$\hbar \frac{dk_x}{dt} = F_x$$

$$\frac{dv_{gx}}{dt} = \frac{1}{\hbar^2} \frac{d^2 E_k}{dk_x^2} F_x$$

Note that:

$$m_{xx}^* \frac{dv_{gx}}{dt} = F_x$$

$$\frac{1}{m_{xx}^*} = \frac{1}{\hbar^2} \frac{d^2 E_k}{dk_x^2}$$

In general:

$$\frac{1}{m_{\mu\nu}^*} = \frac{1}{\hbar^2} \frac{d^2 E_k}{dk_\mu dk_\nu}$$

In three-dimensional k-space, the effective mass is in general a tensor which must be diagonalized to find the principal axis coordinate system and the principal components.

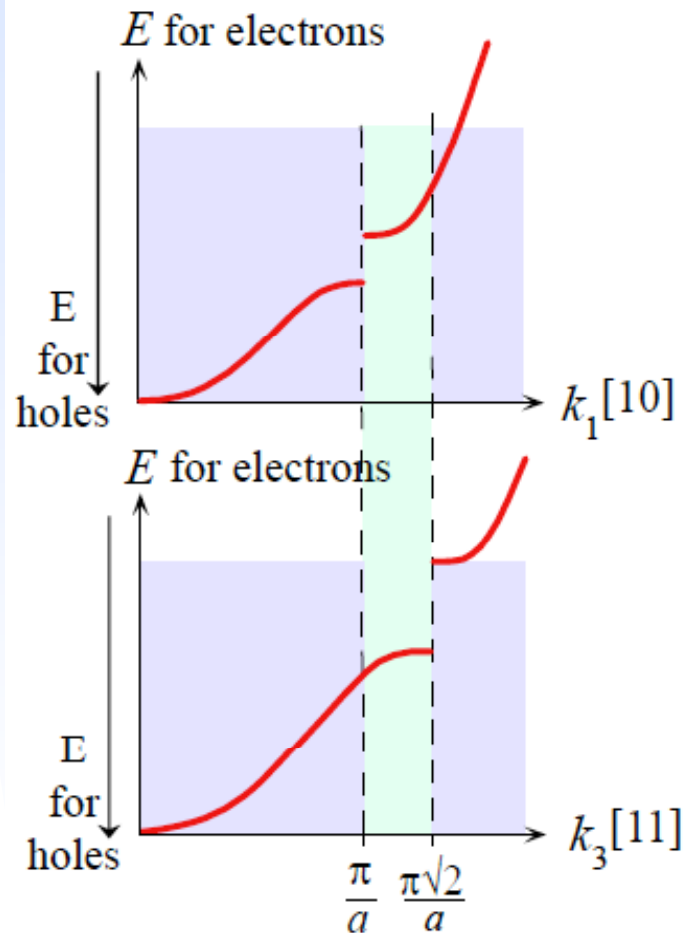
Table 4.2 Effective mass m_e^* of electrons in some metals

| Metal | Ag | Au | Bi | Cu | K | Li | Na | Ni | Pt | Zn |
|---------------------|------|------|-------|------|------|------|-----|----|----|------|
| $\frac{m_e^*}{m_e}$ | 0.99 | 1.10 | 0.047 | 1.01 | 1.12 | 1.28 | 1.2 | 28 | 13 | 0.85 |

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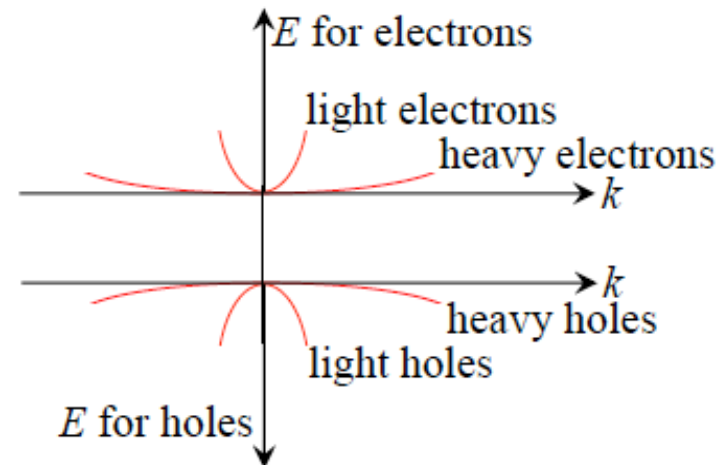
Electron Effective Mass



The effective mass is inversely proportional to the curvature of the E_k function.

At the lowest energies of each band, the effective mass is positive (upward curvature) and assigned to electrons of positive mass and negative charge whose energy increases upward.

At the highest energies of each band, the effective mass is negative (downward curvature) and assigned to holes of positive mass and positive charge whose energy increases downward.



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Comparison of Li ($1s^2 2s^1$) and Si ($1s^2 2s^2 2p^4 3s^2 3p^2$)

Model for Li (BCC):

- *Molecular Orbital Picture*

One-electron wavefunctions are considered as delocalized within the solid. For a given wavefunction, there can be either constructive or destructive interference of neighboring atomic orbitals. The electronic level is determined by the number of occurrences of destructive interference, i.e., by the number of nodes of the wavefunction between the atoms. The collection of N atoms lead to N levels that are continuously distributed in energy. Because there are two spin states per level, $N/2$ levels are filled with N electrons. In addition, the empty $2p$ and $3s$ band states overlap the $2s$ states, leading to a continuous distribution of states from the Fermi level to the vacuum level.

- *Band Picture*

The N electrons fill up one-half the states in the first Brillouin zone in k -space. Electrons can move from the Fermi level to the vacuum level with a large number of infinitesimal energy jumps. When the boundary of the first Brillouin zone is reached, there is a band gap for the given direction of k ; however, by changing its direction in a scattering event, the electron can avoid this gap and cross into the second Brillouin zone with no energy gain.



Comparison of Li ($1s^2 2s^1$) and Si ($1s^2 2s^2 2p^4 3s^2 3p^2$)

Model for Si (diamond cubic):

- *Molecular Orbital Picture*

The four 3s and 3p atomic orbitals hybridize to form four sp^3 molecular orbitals with the ability to accommodate 8 electrons. Because of the localized nature of the electron wavefunctions in the solid, the four molecular orbitals split into bonding and antibonding levels with 4 electrons per atom accommodated in each. In forming the solid from N atoms, the bonding states split into a *valence band* that accommodates $4N$ electrons total and the antibonding states split into the conduction band that also accommodate $4N$ electrons. So the valence band is fully occupied in the solid and the conduction band is empty.

- *Band Picture*

Valence and conduction band states -- $4N$ of each -- can be formed through a linear combination of the localized bonding and antibonding molecular orbitals respectively. The $4N$ electrons fill up the first Brillouin zone in k -space. (There are $2N$ levels in the first Brillouin zone since the Bravais lattice has a 2 atom basis.) At the Brillouin zone boundary there is a band gap, and the lowest energy state in the second zone lies at a higher energy than the highest energy state in the first zone. Thus, the only way to move the electron to the second Brillouin zone is to provide an energy equal to this lowest gap which is simply the *band gap* of Si.

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GENERATION AND RECOMBINATION OF CHARGE

CARRIERS IN SOLAR CELLS;

TRANSPORT MECHANISMS: DRIFT AND

DIFFUSION

February 3, 2011

The University of Toledo, Department of Physics and Astronomy
SSARE, PVIC

Principles and Varieties of Solar Energy (PHYS 4400)
and
Fundamentals of Solar Cells (PHYS 6980)



On today's menu

- generation of free carriers
- recombination of electrons and holes
- Transport:
 - Drift
 - Diffusion

Quiz #2 Tuesday, Feb. 8th



Charge carriers (electrons and holes)

Masses:

$$m_e = 9.11 \times 10^{-31} \text{ kg}$$

$$m_n = 1.67 \times 10^{-27} \text{ kg}$$

$$m_p = 1.67 \times 10^{-27} \text{ kg}$$

$$\text{Electron charge} = -1.602 \times 10^{-19} \text{ C}$$

$$\text{Hole charge} = +1.602 \times 10^{-19} \text{ C}$$

Effective Mass of electrons and holes:

A particle's **effective mass** is the mass it appears to carry in transport in a crystal. Electrons and holes in a crystal respond to electric and magnetic fields almost as if they were particles with a mass dependent on their direction of travel (an effective mass tensor). **Simplified picture:** ignoring crystal anisotropies, electrons and holes behave as free particles in a vacuum, but with a different mass.

[http://en.wikipedia.org/wiki/Effective_mass_\(solid-state_physics\)](http://en.wikipedia.org/wiki/Effective_mass_(solid-state_physics))

| Material | Electron effective mass | Hole effective mass |
|---------------------------|-------------------------|---------------------|
| | Group IV | |
| Si (4.2K) | $1.08 m_e$ | $0.56 m_e$ |
| Ge | $0.55 m_e$ | $0.37 m_e$ |
| | III-V | |
| GaAs | $0.067 m_e$ | $0.45 m_e$ |
| InSb | $0.013 m_e$ | $0.6 m_e$ |
| | II-VI | |
| ZnO | $0.19 m_e$ | $1.21 m_e$ |
| ZnSe | $0.17 m_e$ | $1.44 m_e$ |



Important charge carrier processes in semiconductors

The free electron and hole concentrations in bulk semiconductors can be modified by the processes of generation and recombination, and also by the transport of electrons and holes through drift and diffusion.

Generation: e.g., absorption of a photon generates a free electron and a free hole (an electron-hole pair).

Recombination: can be **radiative**, in which case a photon is emitted as the electron returns to the valence band, or **non-radiative**, in which case the energy associated with the e-h pair is converted to heat, or transferred to another charge carrier (Auger recombination) – non-radiative corresponds to no photon.

Transport is the movement of charge carriers under forces based either on an electric field, or on a concentration gradient:

Drift refers to the motion of charge carriers under the force of an electric field. Motion is typically not “ballistic”, and instead includes the resistive action of scattering.

Diffusion refers to motion of electron and holes due to the presence of a concentration gradient.

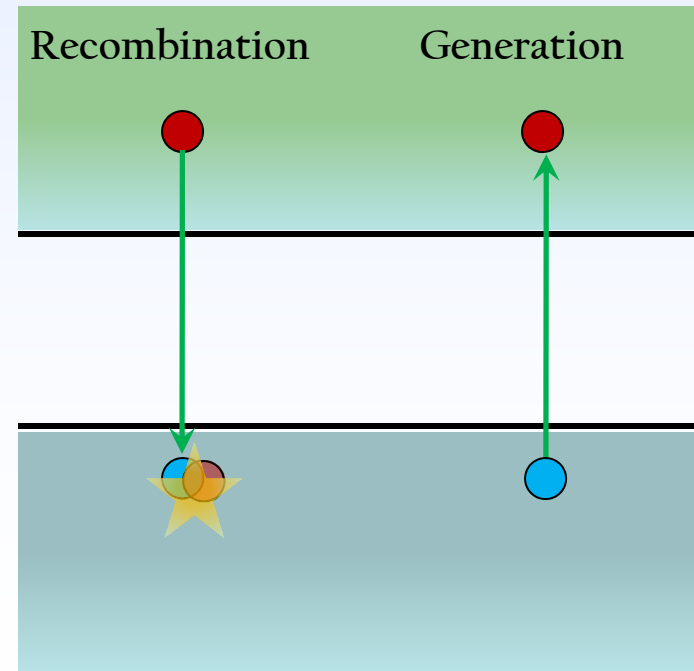


Generation and recombination

Charge carriers move between valence and conduction bands under thermal influence (thermal excitation within the Boltzmann tail of the Fermi-Dirac distribution). In the dark and at equilibrium, the concentration of electrons and holes are unaffected by these processes.

Generation, under influence of light absorption for example, promotes electrons from the valence band to the conduction band, resulting in a new free electron in the CB, and a new hole in the VB.

Recombination is essentially the reverse process, in which an electron returns to the valence band, giving up its electronic potential energy to a photon, or a third carrier, or to phonons.



Absorption of light

Light incident on a semiconductor consist of photons with energy $E = h\nu = hc/\lambda$. Photons interact with the semiconductor depending on their energy:

$E_{\text{photon}} < E_g$: Photons with energy below the band gap energy are transmitted through the material;

$E_{\text{photon}} = E_g$: These photons have sufficient energy to be absorbed in a band-to-band transition, and generate an electron-hole pair. Absorption of these photons will be relatively weak.

$E_{\text{photon}} > E_g$: Photons with significantly greater energy than the semiconductor's bandgap are relatively strongly absorbed, and generate electron-hole pairs with initial excess kinetic energy. This excess kinetic energy is, in general, quickly lost to the lattice as phonons).



Absorption of light – the generation rate

The generation rate quantifies the number of electron-hole pairs created per unit time. As the light enters and travels through the semiconductor, the intensity of the light drops exponentially as the photons are converted to electron-hole pairs by the process of “photogeneration”:

$$I = I_0 e^{-\alpha x}$$

where α is the absorption coefficient typically in cm^{-1} , and x is the distance into the material. I_0 is the light intensity just inside the surface of the semiconductor.

Since each photon absorbed generates an e-h pair, this exponential decay also mimics the generation of carriers as a function of depth.

The generation rate, G , is given by:

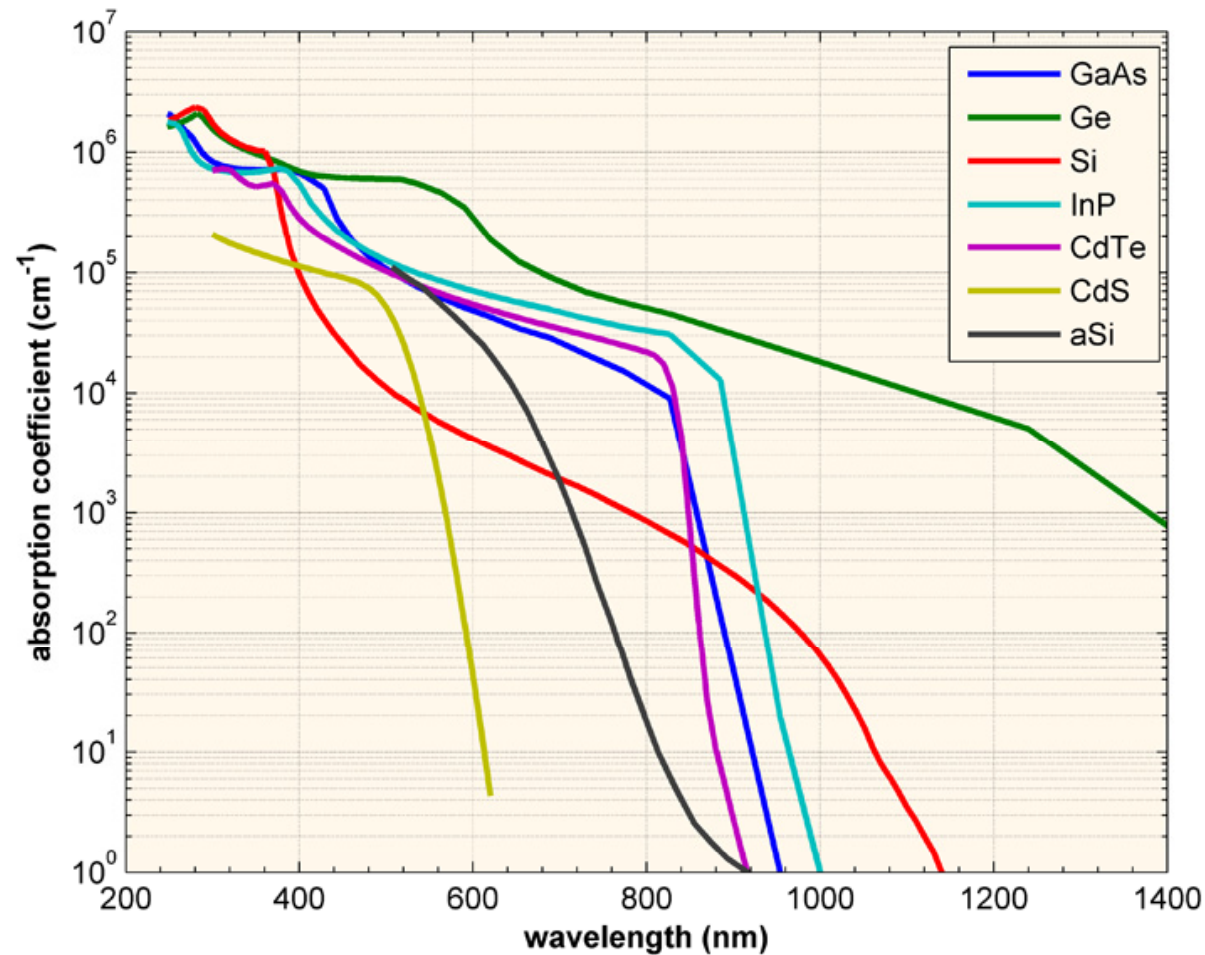
$$G = \alpha N_0 e^{-\alpha x}$$

where N_0 is the photon flux at the surface (photons/unit-area/sec), α is absorption coefficient, and x is the distance into the material.



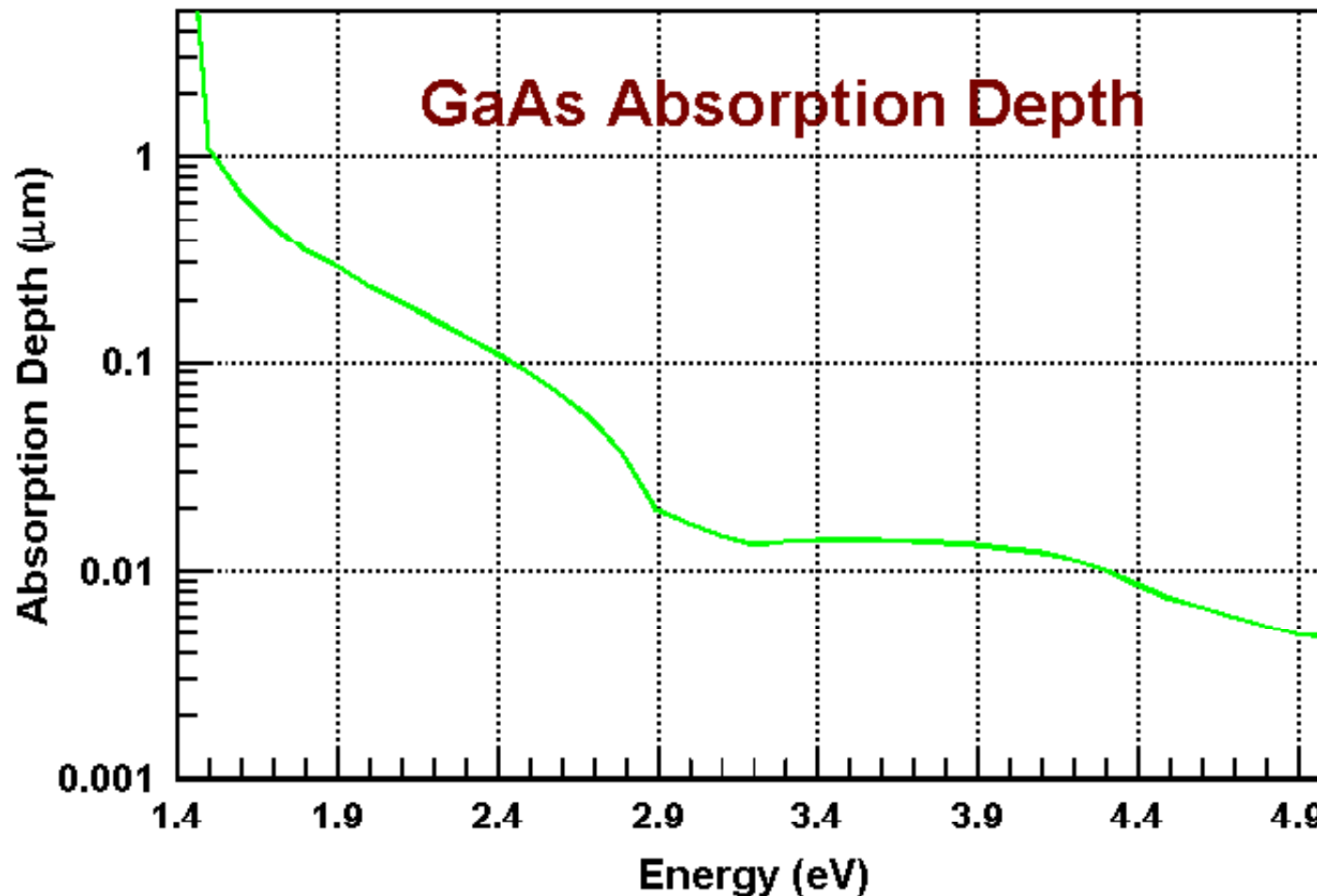
Absorption coefficient

Generation occurs in PV cells by absorption of light, and the formation of electron-hole pairs. The absorption coefficient, α , in units of cm^{-1} , provides a measure of the strength of the light absorption at a given photon energy.



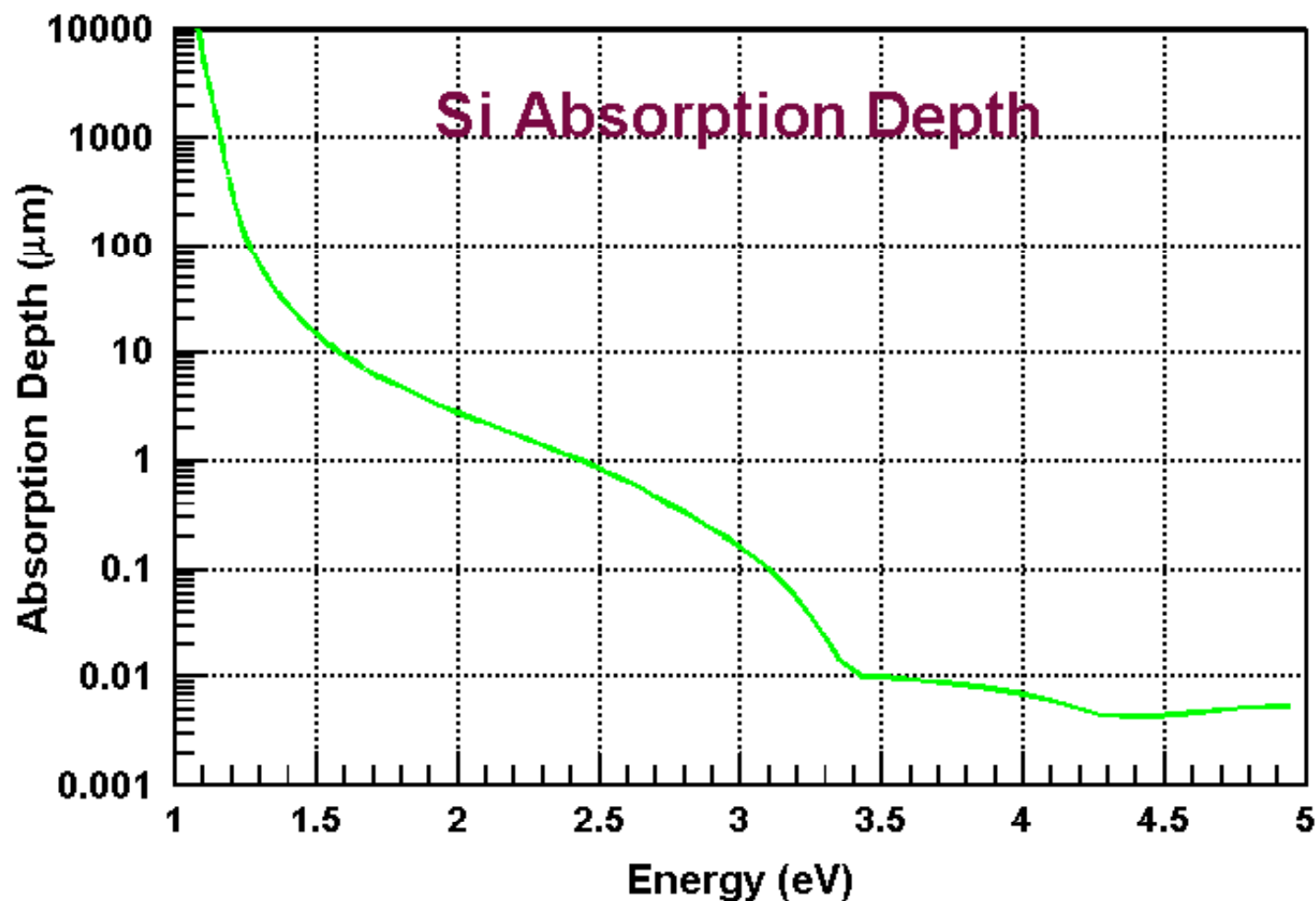
Absorption *depth*

The absorption depth for a materials is photon-energy-dependent, and is simply the inverse of the absorption coefficient. I.e., it is the depth at which the intensity of the light has dropped to a value of $(1/e)*I_0(\lambda)$.



Absorption *depth*

The absorption depth for a materials is photon-energy-dependent, and is simply the inverse of the absorption coefficient. I.e., it is the depth at which the intensity of the light has dropped to a value of $(1/e) \cdot I_0(\lambda)$.



Recombination of electrons and holes in a semiconductor

Photons incident on the surface of a semiconductor will be either reflected from the top surface, absorbed, or transmitted. For PV, reflection and transmission are typically considered loss mechanisms (photons which are not absorbed do not generate power). An absorbed photon will raise an electron from the valence band to the conduction band (this process is called *generation*). A key factor in determining if a photon is absorbed or transmitted is the energy of the photon.

An electron which exists in the conduction band is in a meta-stable state and will eventually fall back to a lower energy position in the valence band. It must move back into an empty valence band state and consequently, when the electron falls back down into the valence band, it effectively removes a hole. This process is called *recombination*. There are three basic types of recombination in the bulk of a single-crystal semiconductor. These are:

- (1) Radiative (band-to-band) recombination
- (2) Auger recombination
- (3) Shockley-Read-Hall (SRH) recombination



Free carriers (free electrons and holes)

Free carriers -- consisting of electrons, holes, or both – are able to carry current in a semiconductor material or solar cell.

In contrast, trapped carriers are bound to a specific impurity atom, defect (such as a vacancy) in the crystal, or bound to a specific surface state. Trapped carriers are typically not in the valence band, and cannot carry current.

Free carriers are subject to move under the mechanisms of drift (as in an electric field, with force of qE where q is the electron charge and E is the electric field strength), and of diffusion.



Drift of free carriers in solar cells

Drift refers to the motion of a charged particle within an electric field (typically DC and in a steady direction);

The **drift velocity** is the average velocity that a particle, such as an electron, attains due to an electric field. In general, an electron will 'rattle around' in a conductor at the Fermi velocity randomly. An applied electric field will give this random motion a small net velocity in one direction.

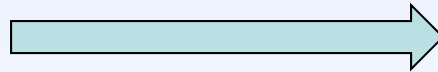
http://en.wikipedia.org/wiki/Drift_velocity



Diffusion of free carriers in solar cells

Diffusion describes the spread of particles through random motion from regions of higher concentration to regions of lower concentration. The time dependence of the statistical distribution in space is given by the diffusion equation. The concept of diffusion is tied to that of mass transfer driven by a concentration gradient, but diffusion can still occur when there is no concentration gradient (but there will be no net flux).

<http://en.wikipedia.org/wiki/Diffusion>



Diffusion current is a current in a semiconductor caused by the diffusion of charge carriers (holes and/or electrons). Diffusion current can be in the same or opposite direction of a drift current.

At equilibrium (i.e., in the dark) in a p-n junction, the forward diffusion current in the depletion region is balanced with a reverse drift current, so that the net current is zero.



Current based on fundamental transport mechanisms

For compositionally invariant material, at a uniform temperature, the current density (A/cm²) due to drift and diffusion of electrons and holes are given by:

$$J_n(r) = qD_n \nabla n + q\mu_n En$$

$$J_p(r) = qD_p \nabla p + q\mu_p Ep$$

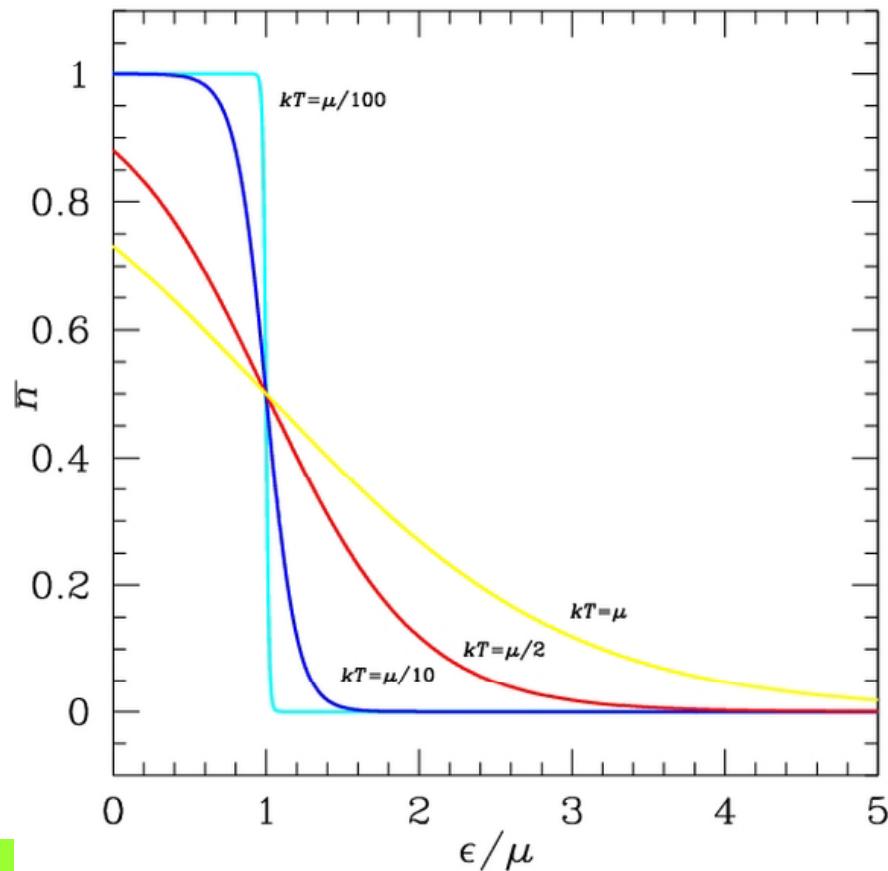
where q is the carrier charge ($-e$, or $+e$), $D_{n,p}$ are the diffusion coefficients (cm² s⁻¹), ∇n and ∇p are the concentration gradients for electron and holes (cm⁻⁴), $\mu_{n,p}$ are the mobilities for electrons and holes (cm² V⁻¹ s⁻¹), E is the electric field strength (V cm⁻¹), and n, p are the electron and hole concentrations (cm⁻³).



Fermi-Dirac statistics

$$\bar{n}_i = \frac{1}{e^{(\varepsilon_i - \mu)/kT} + 1}$$

where k is Boltzmann's constant, T is the absolute temperature, ε_i is the energy of the single-particle state i , and μ is the chemical potential. At $T = 0$, the chemical potential is equal to the Fermi energy. For the case of electrons in a semiconductor, is also called the Fermi level.



The periodic table

| | | | | | | | | | | | | | | | | | |
|--|--|---|---|--|--|--|---|--|--|--|--|---|---|---|--|--|---|
| 1 IA | | | | | | | | | | | | | | | | | 18 VIIIA |
| 1 H 1 1.008 Hydrogen | 2 He 2 4.00 Helium | | | | | | | | | | | | | | | | |
| 2 Li 3 6.94 Lithium | 2 Be 4 9.01 Beryllium | | | | | | | | | | | | | | | | |
| 3 Na 11 22.99 Sodium | 2 Mg 12 24.31 Magnesium | 13 B 5 10.81 Boron | 14 C 6 12.01 Carbon | 15 N 7 14.01 Nitrogen | 16 O 8 16.00 Oxygen | 17 F 9 19.00 Fluorine | 18 Ne 10 20.18 Neon | | | | | | | | | | |
| 4 K 19 39.10 Potassium | 2 Ca 20 40.08 Calcium | 3 Sc 21 44.96 Scandium | 4 Ti 22 47.88 Titanium | 5 V 23 50.94 Vanadium | 6 Cr 24 52.00 Chromium | 7 Mn 25 54.94 Manganese | 8 Fe 26 55.85 Iron | 9 Co 27 58.93 Cobalt | 10 Ni 28 58.69 Nickel | 11 Cu 29 63.55 Copper | 12 Zn 30 65.39 Zinc | 13 Ga 31 69.72 Gallium | 14 Ge 32 72.61 Germanium | 15 As 33 74.92 Arsenic | 16 Se 34 78.96 Selenium | 17 Br 35 79.90 Bromine | 18 Kr 36 83.80 Krypton |
| 5 Rb 37 85.47 Rubidium | 2 Sr 38 87.62 Strontium | 3 Y 39 88.91 Yttrium | 4 Zr 40 91.22 Zirconium | 5 Nb 41 92.91 Niobium | 6 Mo 42 95.94 Molybdenum | 7 Tc 43 (97.9) Technetium | 8 Ru 44 101.07 Ruthenium | 9 Rh 45 102.91 Rhodium | 10 Pd 46 106.42 Palladium | 11 Ag 47 107.87 Silver | 12 Cd 48 112.41 Cadmium | 13 In 49 114.82 Indium | 14 Sn 50 118.71 Tin | 15 Sb 51 121.76 Antimony | 16 Te 52 127.60 Tellurium | 17 I 53 126.90 Iodine | 18 Xe 54 131.29 Xenon |
| 6 Cs 55 132.91 Cesium | 2 Ba 56 137.33 Barium | 3 La 57 138.91 Lanthanum | 4 Hf 72 178.49 Hafnium | 5 Ta 73 180.95 Tantalum | 6 W 74 183.85 Tungsten | 7 Re 75 186.21 Rhenium | 8 Os 76 190.2 Osmium | 9 Ir 77 192.22 Iridium | 10 Pt 78 195.08 Platinum | 11 Au 79 196.97 Gold | 12 Hg 80 200.59 Mercury | 13 Tl 81 204.38 Thallium | 14 Pb 82 207.2 Lead | 15 Bi 83 208.98 Bismuth | 16 Po 84 (209) Polonium | 17 At 85 (210) Astatine | 18 Rn 86 (222) Radon |
| 7 Fr 87 223.02 Francium | 2 Ra 88 226.03 Radium | 3 Ac 89 227.03 Actinium | 4 Rf 104 (261) Rutherfordium | 5 Db 105 (262) Dubnium | 6 Sg 106 (263) Seaborgium | 7 Bh 107 (262) Bohrium | 8 Hs 108 (265) Hassium | 9 Mt 109 (266) Meitnerium | 10 Unnamed Discovery 110 Nov. 1994 | 11 Unnamed Discovery 111 Nov. 1994 | 12 Unnamed Discovery 112 1996 | 13 Unnamed Discovery 114 1999 | 14 Unnamed Discovery 116 1999 | 15 Unnamed Discovery 118 1999 | 16 Unnamed Discovery 119 1999 | 17 Unnamed Discovery 120 1999 | 18 Unnamed Discovery 121 1999 |



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LANTHANIDES

ACTINIDES

| | | | | | | | | | | | | | |
|--------------------------------------|---|--|--|---------------------------------------|--|---|---------------------------------------|---|--|---------------------------------------|--|--|--|
| Ce 58 140.12 Cerium | Pr 59 140.91 Praseodymium | Nd 60 144.24 Neodymium | Pm 61 (145) Promethium | Sm 62 150.36 Samarium | Eu 63 152.97 Europium | Gd 64 157.25 Gadolinium | Tb 65 158.93 Terbium | Dy 66 162.50 Dysprosium | Ho 67 164.93 Holmium | Er 68 167.26 Erbium | Tm 69 168.93 Thulium | Yb 70 173.04 Ytterbium | Lu 71 174.97 Lutetium |
| Th 90 232.04 Thorium | Pa 91 231.04 Protactinium | U 92 238.03 Uranium | Np 93 237.05 Neptunium | Pu 94 (240) Plutonium | Am 95 243.06 Americium | Cm 96 (247) Curium | Bk 97 (248) Berkelium | Cf 98 (251) Californium | Es 99 252.08 Einsteinium | Fm 100 257.10 Fermium | Md 101 (257) Mendelevium | No 102 259.10 Nobelium | Lr 103 262.11 Lawrencium |

Common elemental components of semiconductors

| | | | | | | | |
|-----------------------------|----------------------------|----------------------------|----------------------------|-----------------------------|----------------------------|----------------------------|----------------------------|
| | | | | | | | VIIIA |
| | | | | | | | ² He 4.003 |
| | | IIIA | IVA | VA | VIA | VIIA | |
| | | ⁵ B 10.811 | ⁶ C 12.011 | ⁷ N 14.007 | ⁸ O 15.999 | ⁹ F 18.998 | ¹⁰ Ne 20.183 |
| IB | IIB | ¹³ Al 26.982 | ¹⁴ Si 28.086 | ¹⁵ P 30.974 | ¹⁶ S 32.064 | ¹⁷ Cl 35.453 | ¹⁸ Ar 39.948 |
| ²⁹ Cu 63.54 | ³⁰ Zn 65.37 | ³¹ Ga 69.72 | ³² Ge 72.59 | ³³ As 74.922 | ³⁴ Se 78.96 | ³⁵ Br 79.909 | ³⁶ Kr 83.80 |
| ⁴⁷ Ag 107.870 | ⁴⁸ Cd 112.40 | ⁴⁹ In 114.82 | ⁵⁰ Sn 118.69 | ⁵¹ Sb 121.75 | ⁵² Te 127.60 | ⁵³ I 126.904 | ⁵⁴ Xe 131.30 |
| ⁷⁹ Au 196.967 | ⁸⁰ Hg 200.59 | ⁸¹ Tl 204.37 | ⁸² Pb 207.19 | ⁸³ Bi 208.980 | ⁸⁴ Po (210) | ⁸⁵ At (210) | ⁸⁶ Rn (222) |



Electron configuration of the elements

DIVISION

| | | | | | |
|--|---|---|---|--|---|
| | | | | | <div>2 He $1s^2$ helium 4.003</div> |
| 3A | 4A | 5A | 6A | 7A | |
| <div>5 B $[\text{He}]2s^2 2p^1$ boron 10.81</div> | <div>6 C $[\text{He}]2s^2 2p^2$ carbon 12.01</div> | <div>7 N $[\text{He}]2s^2 2p^3$ nitrogen 14.01</div> | <div>8 O $[\text{He}]2s^2 2p^4$ oxygen 16.00</div> | <div>9 F $[\text{He}]2s^2 2p^5$ fluorine 19.00</div> | <div>10 Ne $[\text{He}]2s^2 2p^6$ neon 20.18</div> |
| <div>13 Al $[\text{Ne}]3s^2 3p^1$ aluminum 26.98</div> | <div>14 Si $[\text{Ne}]3s^2 3p^2$ silicon 28.09</div> | <div>15 P $[\text{Ne}]3s^2 3p^3$ phosphorus 30.97</div> | <div>16 S $[\text{Ne}]3s^2 3p^4$ sulfur 32.07</div> | <div>17 Cl $[\text{Ne}]3s^2 3p^5$ chlorine 35.45</div> | <div>18 Ar $[\text{Ne}]3s^2 3p^6$ argon 39.95</div> |

<http://www.sciencegeek.net/tables/LosAlamosperiodictableColor.pdf>



Special talk Friday

Friday, Feb. 4, 2011

3:00 – 3:40 pm, R1, Conf. Rm B (1st floor)

Surface Recombination Velocity (in Solar Cells)
Carmen Cioc

