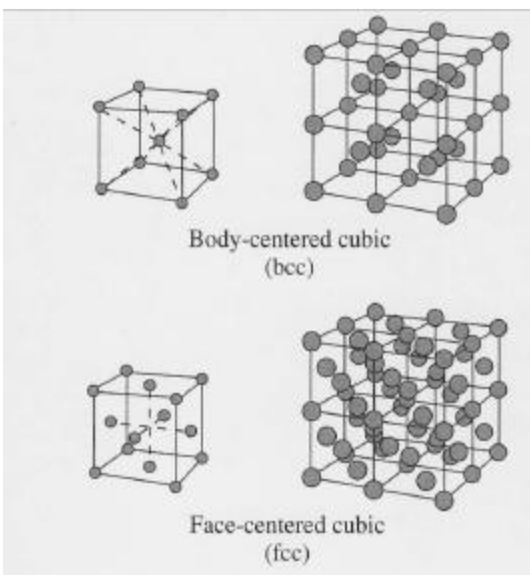
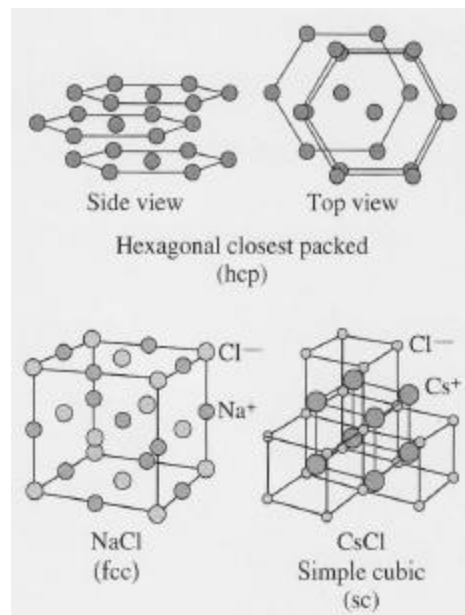
Lecture 12 Topics

- Crystal Structures
- Energy bands
  - In a 4-atom crystal
  - in an N-atom crystal
  - Conductors, insulators, and semiconductors
- Conduction
  - Drift velocity
  - Collision time
  - Conductivity

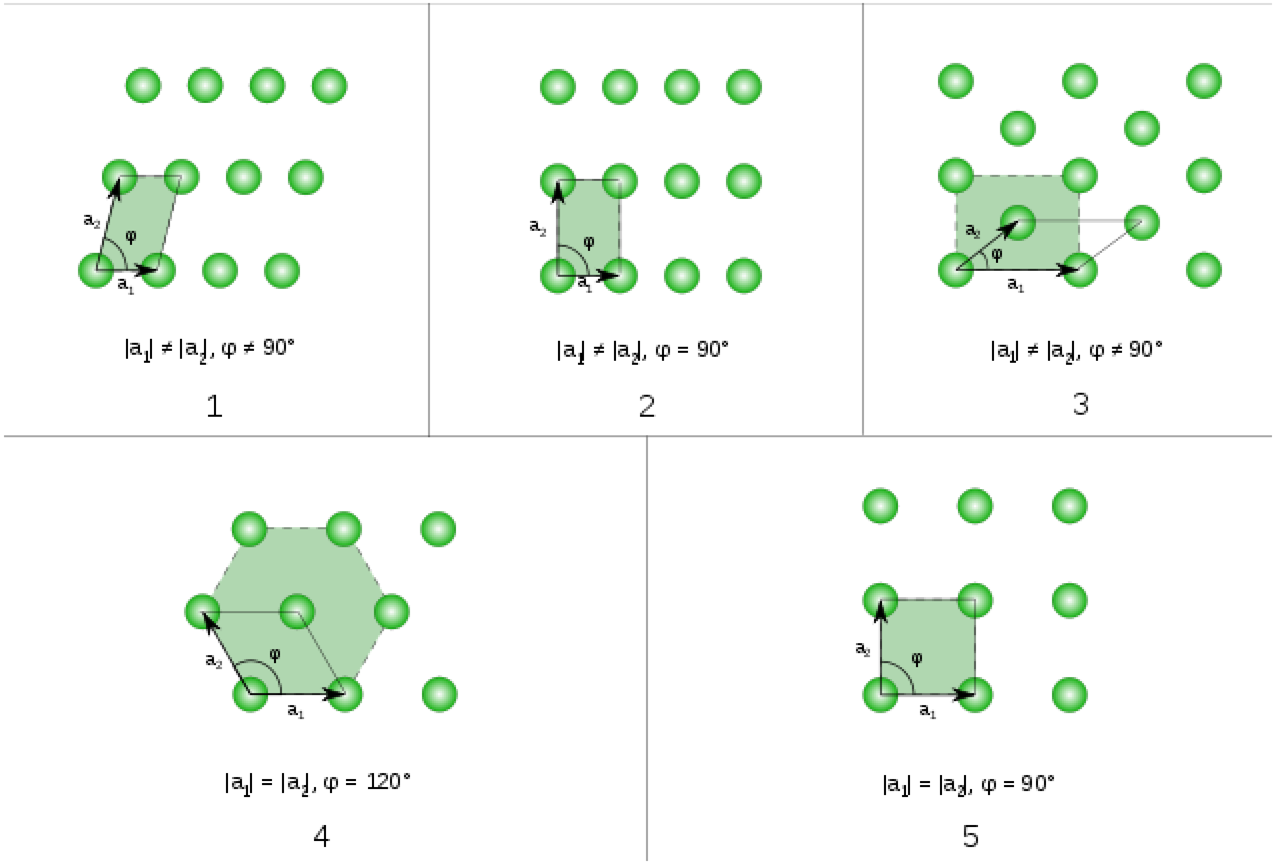
Crystal Lattice Types

- A very large number of atoms are bonded together to create a lattice structure.
- Lattice: a structural unit that repeats to fill space without gap and without overlap
- 14 possible lattice types:



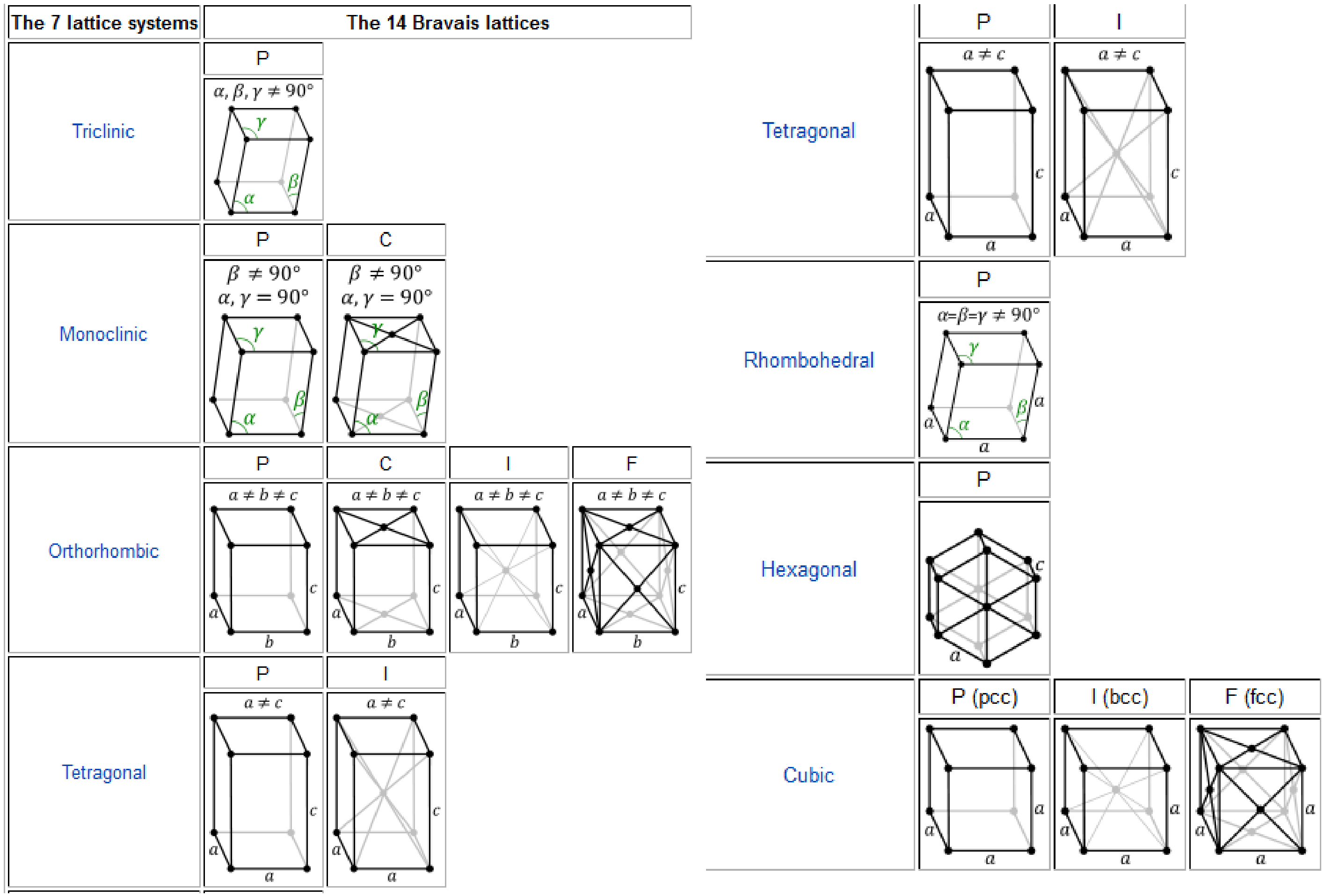


2 dimensional lattice types



Lattice: a structural unit that repeats to fill space without gap and without overlap

3 dimensional lattice types

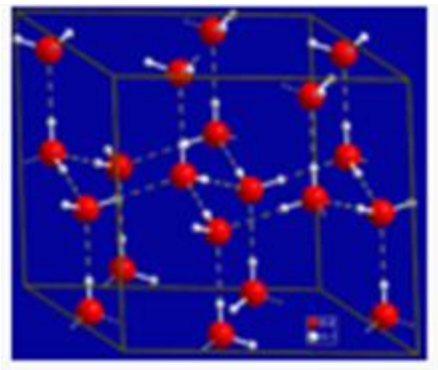


Solid Types

	Bond types	Nature of Bonding	Conductivity	Malleability	Strength
Molecular solid	Inter-molecular bond	Dipole/dipole interaction			
Ionic solid	Ionic bond	Electrostatic			
Covalent solid	Covalent bond	Electron sharing by neighboring atoms			
Metallic solid	Metallic bond	Electron sharing by N atoms			

Identifying sold types

A



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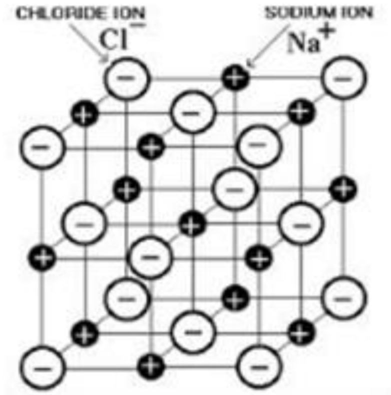

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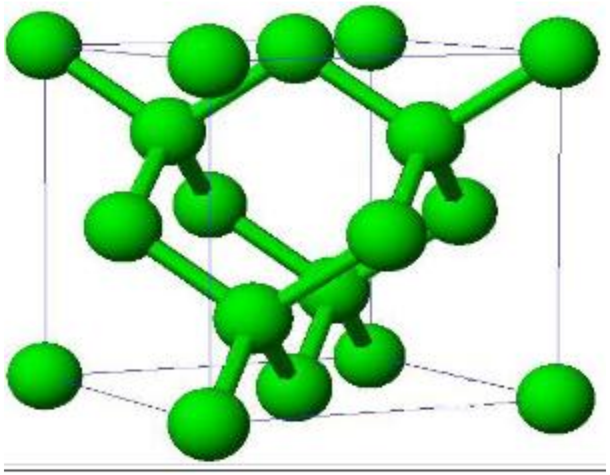

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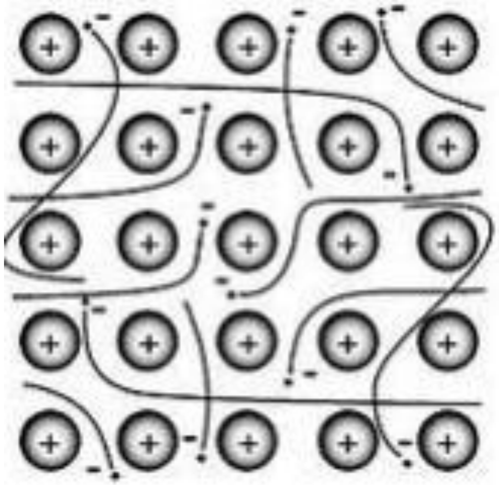
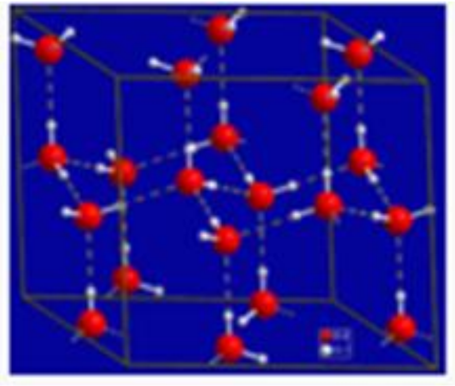
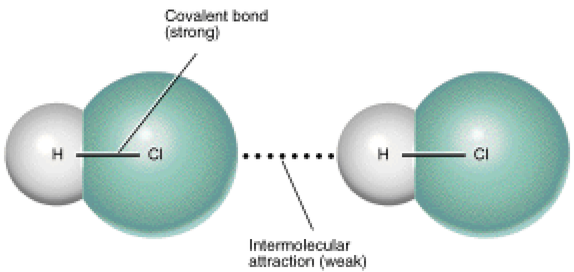




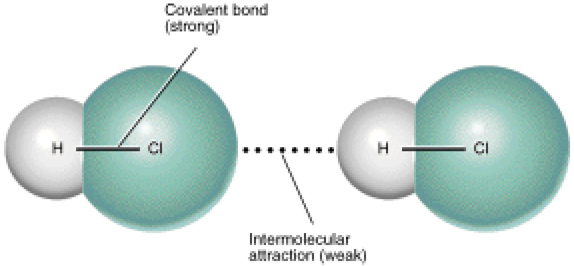
Solid Types

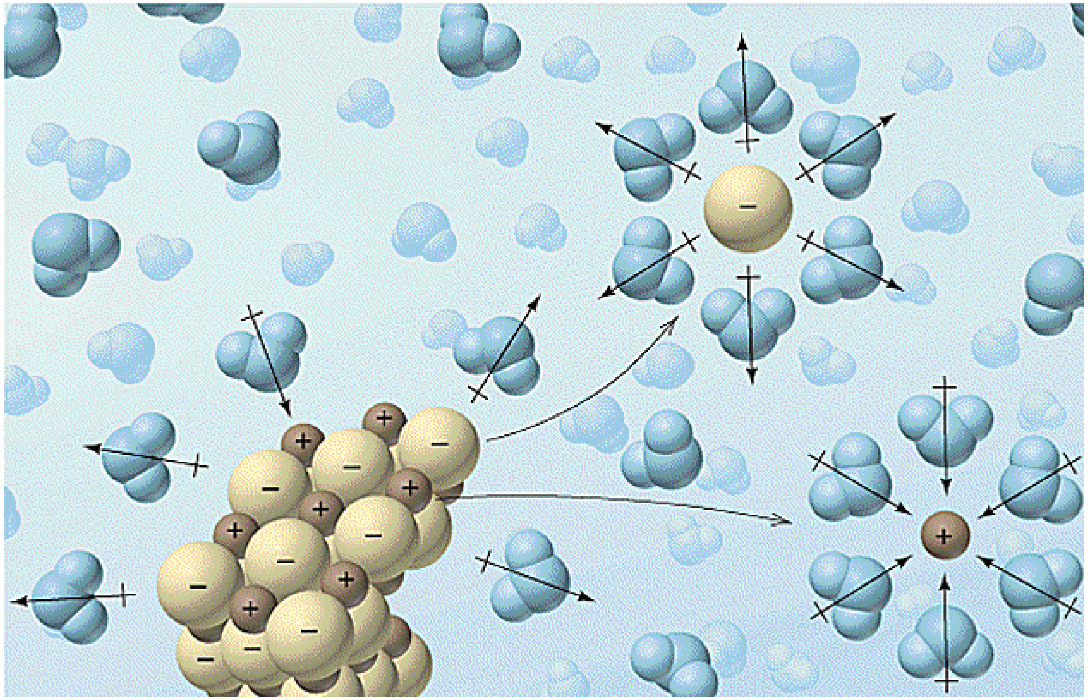
			Conductivity	Malleability (Breakability)	Strength
Molecular solid	Inter molecular bond	Electrostatic due to Dipole/dipole interaction	no	breaks	Very weak
Ionic solid	Ionic bond	Electrostatic	no	breaks	Weak
Covalent solid	Covalent bond	Electron sharing by neighboring atoms	no	no	Strong
Metallic solid	Metallic bond	Electron sharing by N atoms	Yes (electrons free to move)	yes	Strong

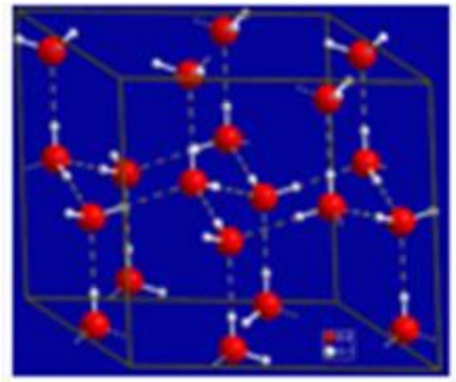
Permanent dipole



Dipole/dipole interaction







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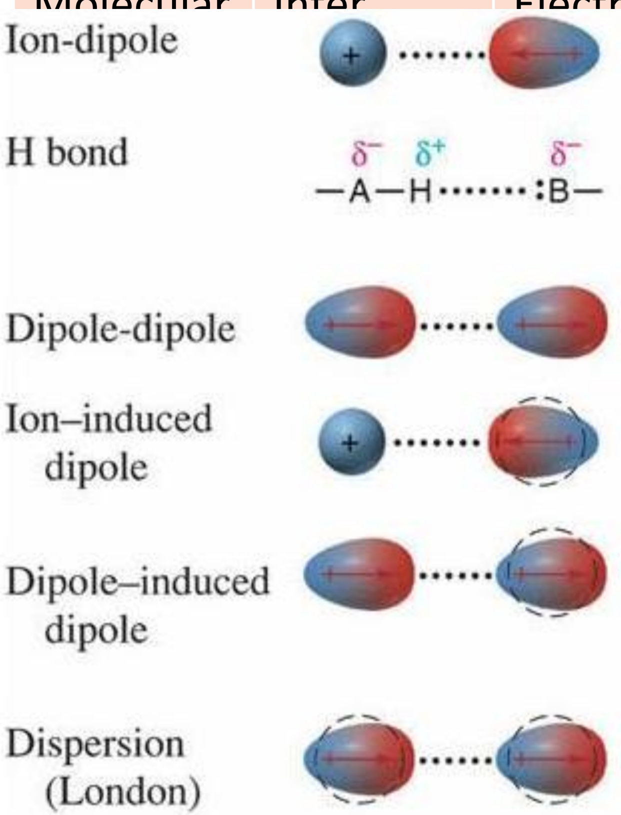

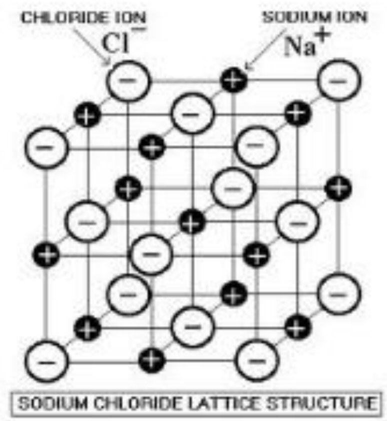

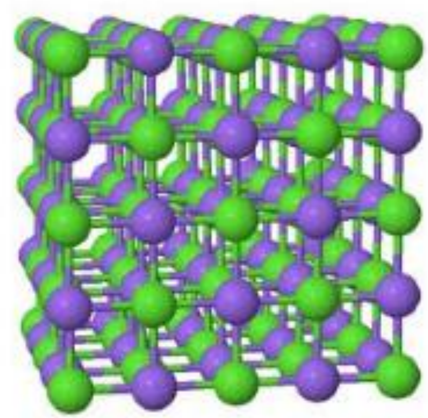

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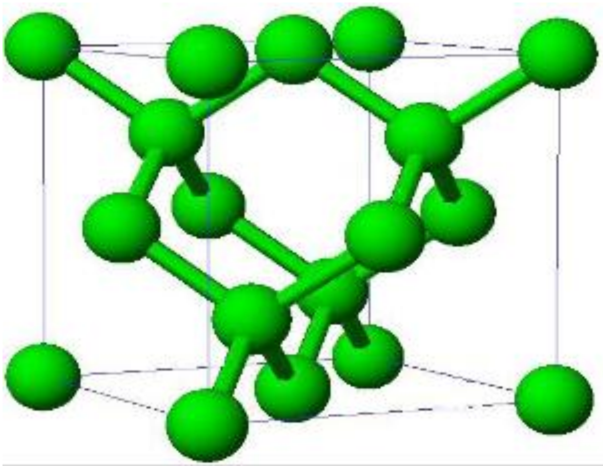

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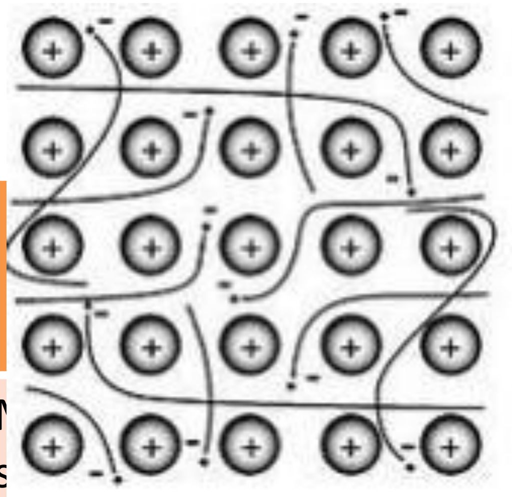

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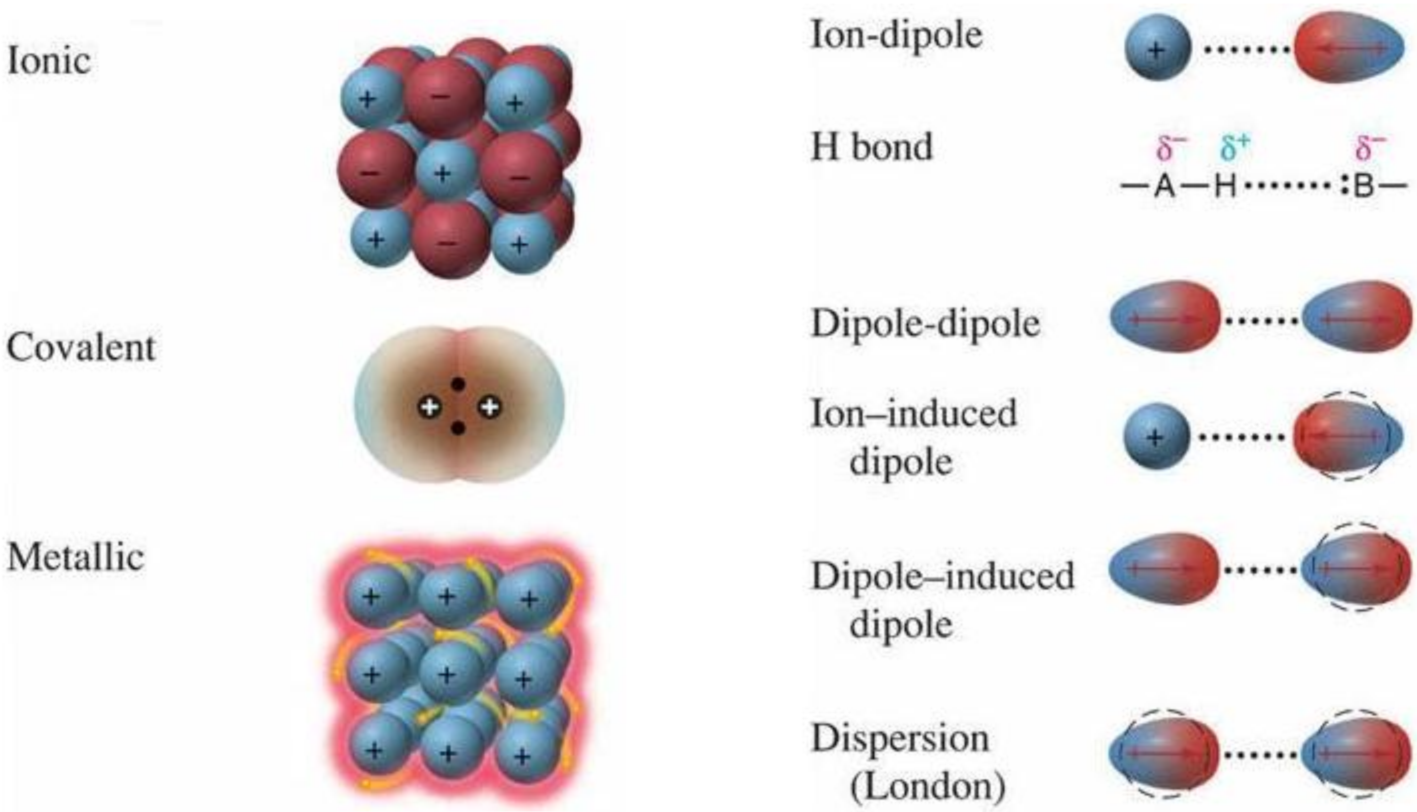
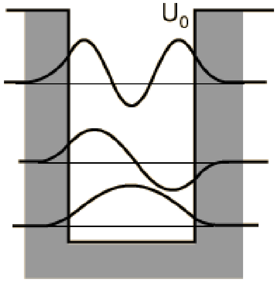
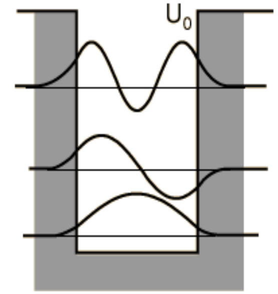
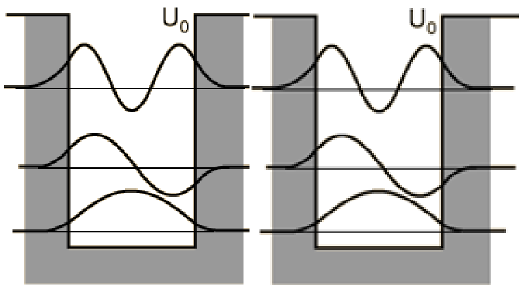
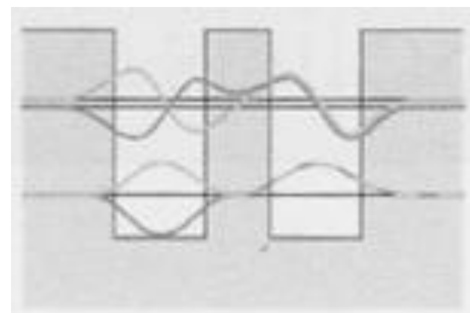

Ionic
Covalent
Metallic
Ion-dipole
H bond
δ⁻ δ⁺ δ⁻
—A—H·······:B—
Dipole-dipole
Ion–induced dipole
Dipole–induced dipole
Dispersion (London)

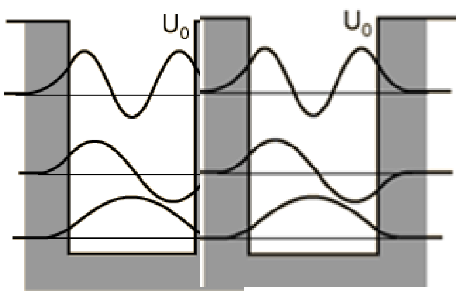
When two atoms are together

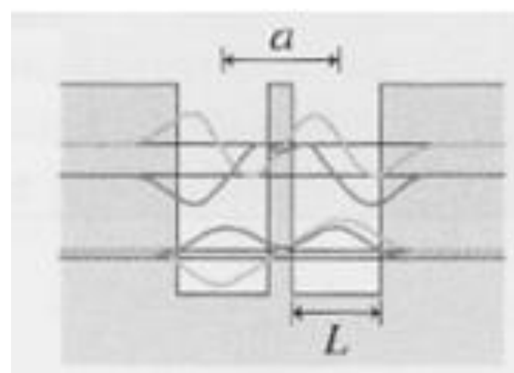




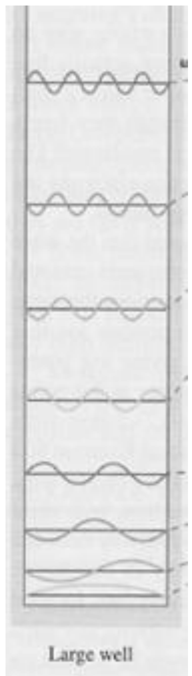








When 4 atoms are together



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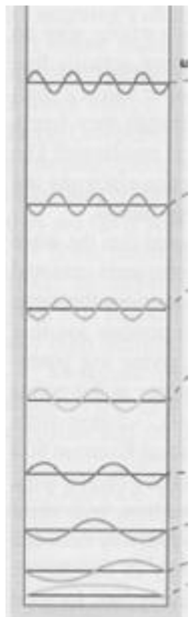
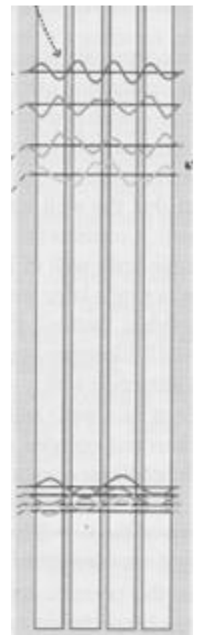
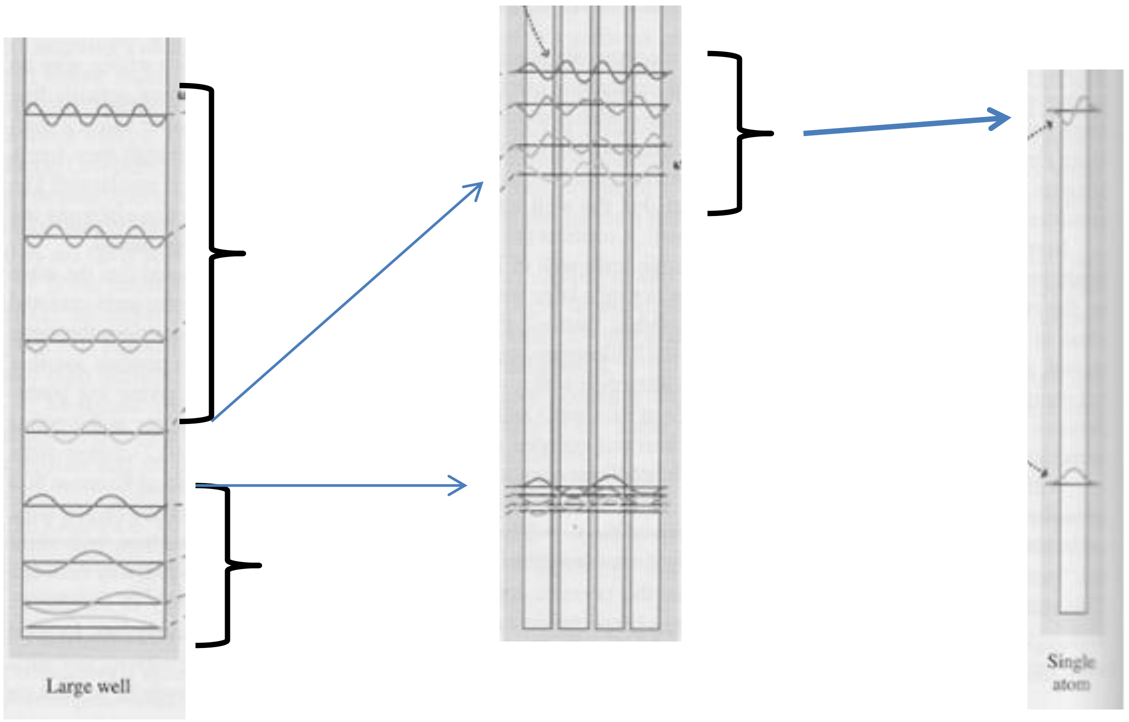


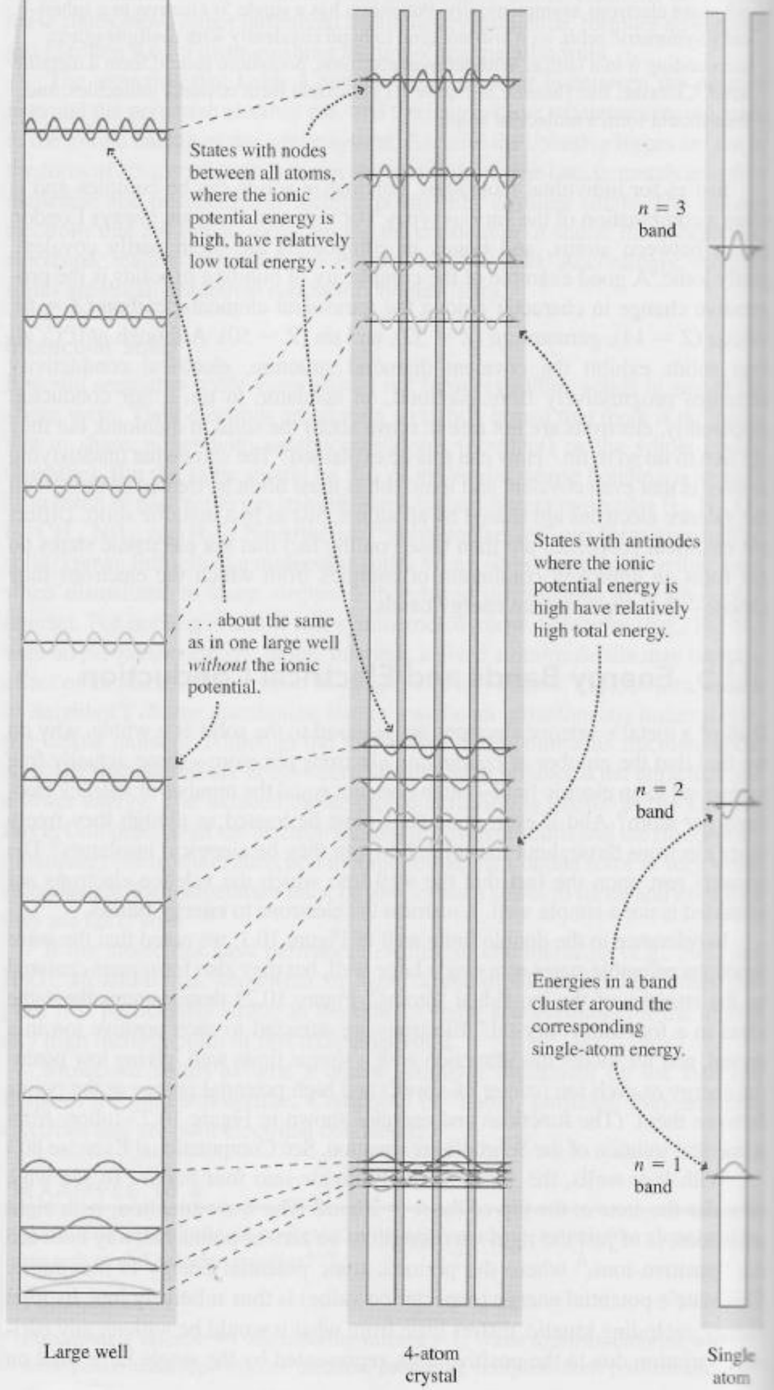
Large well



Single atom

When 4 atoms are together



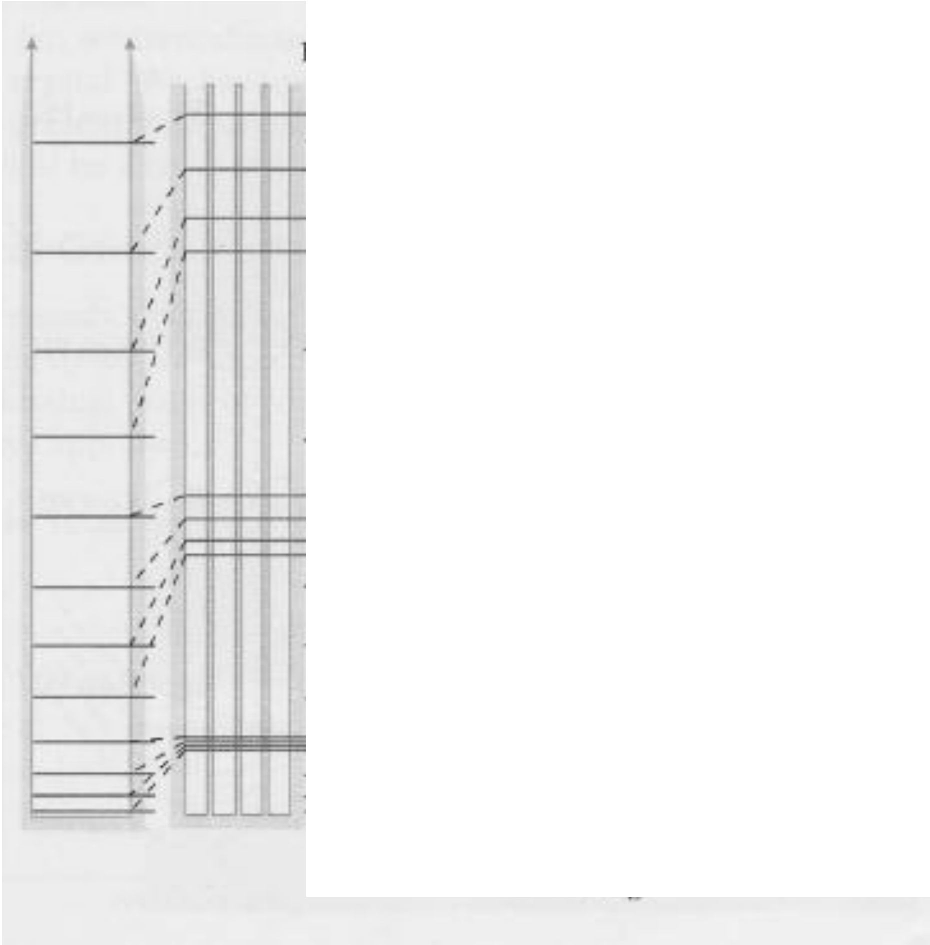


States with nodes between all atoms, where the ionic potential energy is high, have relatively low total energy . . .
. . . about the same as in one large well *without* the ionic potential.
States with antinodes where the ionic potential energy is high have relatively high total energy.
Energies in a band cluster around the corresponding single-atom energy.
n = 3 band
n = 2 band
n = 1 band
Large well
4-atom crystal
Single atom

Comparing energy bands vs. free particle solution

Free particle solution:

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



Large well   4-atom well

Comparing energy bands vs. free particle solution

Free particle solution:

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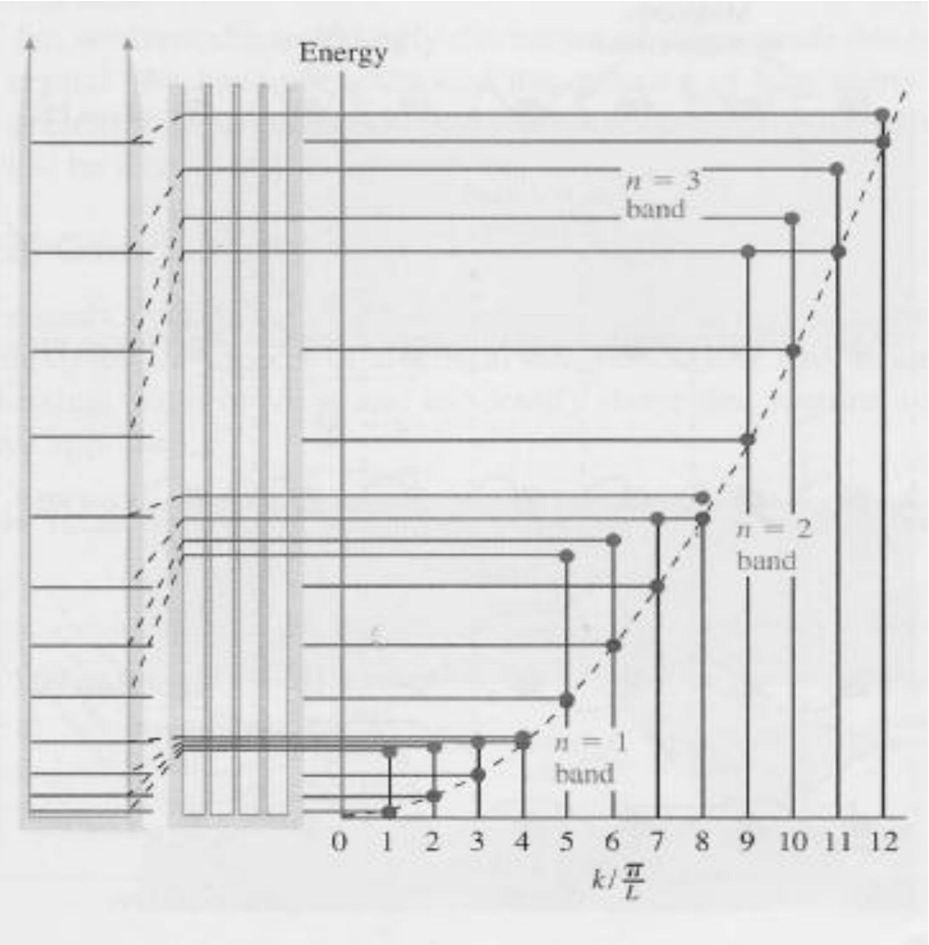
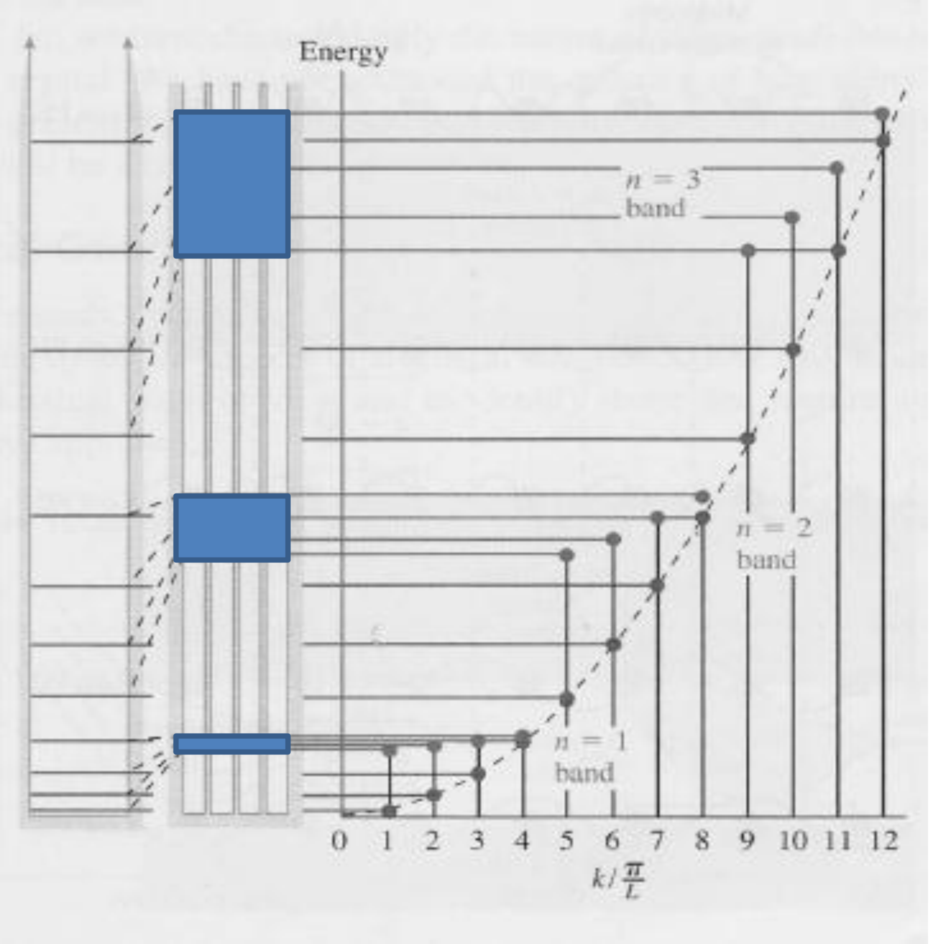


Large well   4-atom well

Comparing energy bands vs. free particle solution

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



Large well   4-atom well

When N atoms come together

- There will be energy bands
- Each energy band corresponds to one of the energy levels in a single atom
-Each energy band has N states
-If N is large, then energy levels inside the band can be considered continuous
-Top of energy band (n) has n antinodes per atom, nN antinodes overall.
- Energy gap occurs at:

$$a = n\frac{1}{2}\lambda$$

$$\frac{2\pi}{\lambda} = \frac{n\pi}{a}$$

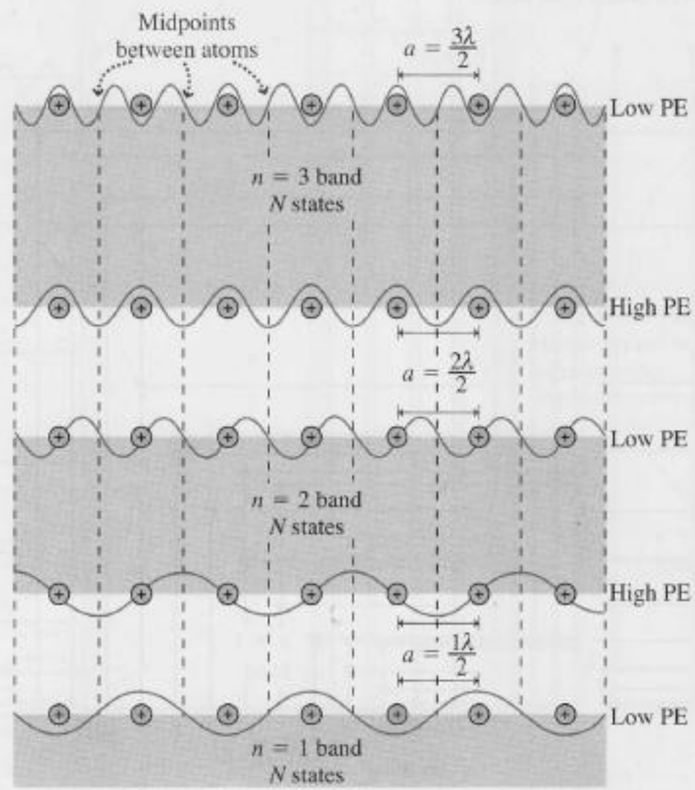


Figure 10.25 Band gaps occur when $a = n\lambda/2$ or $k = n\pi/a$. Top-of-the-band states are zero between atoms, where the potential energy is high, whereas bottom-of-the-band states are large there.

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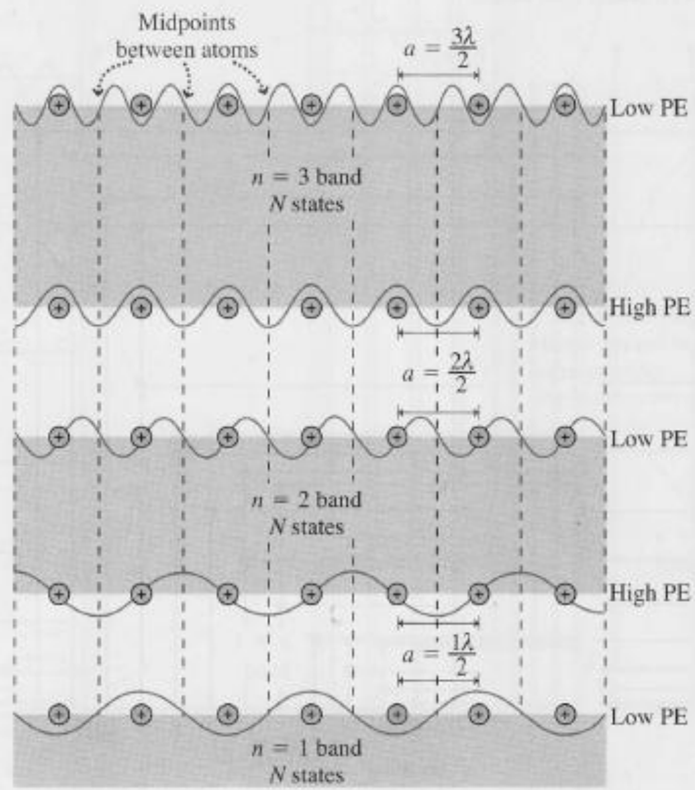
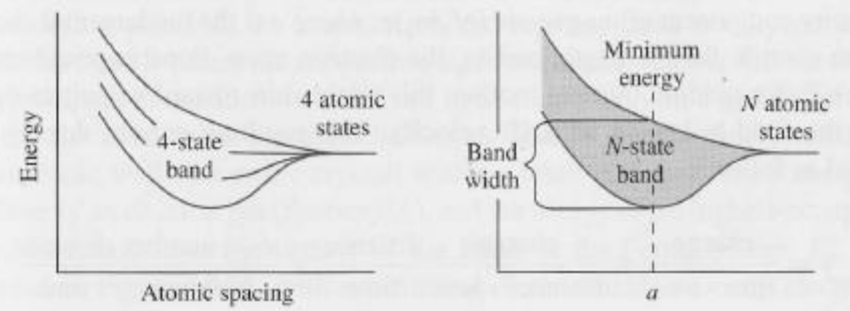


Energy band width

- Depends on the atomic spacing in a crystal.
- Band width is largest at the spacing that makes the crystal most stable.

Figure 10.26 Behavior of allowed electron states as atomic spacing varies.



Energy band width

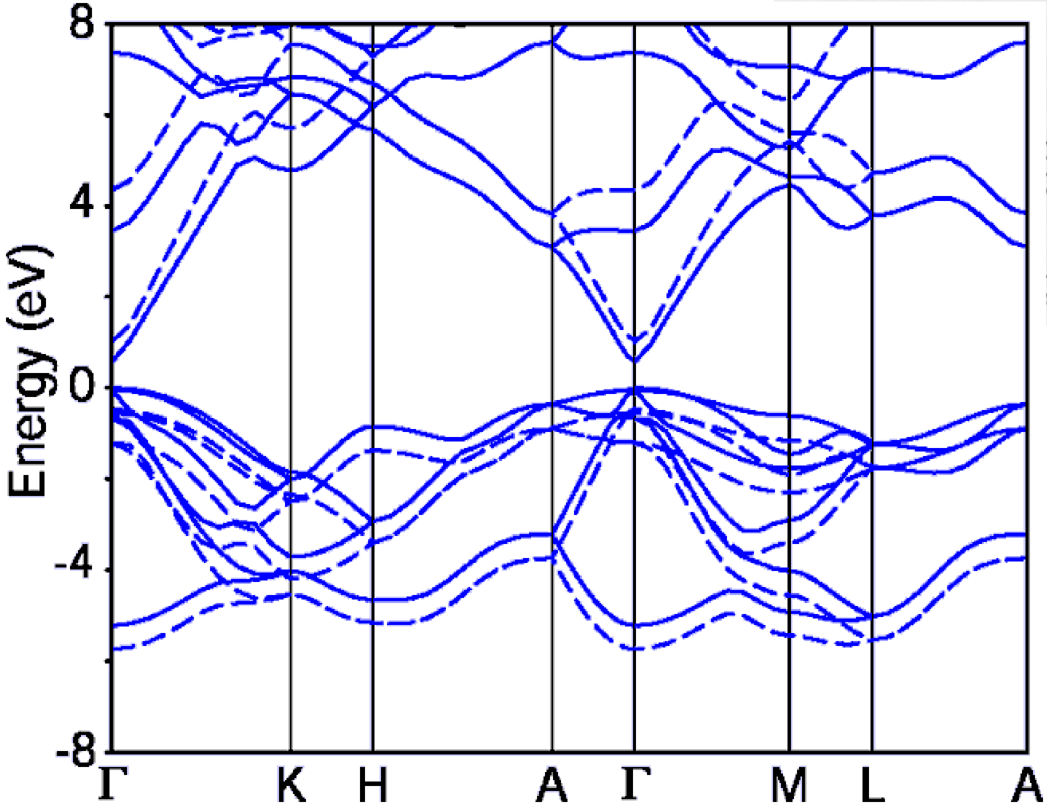
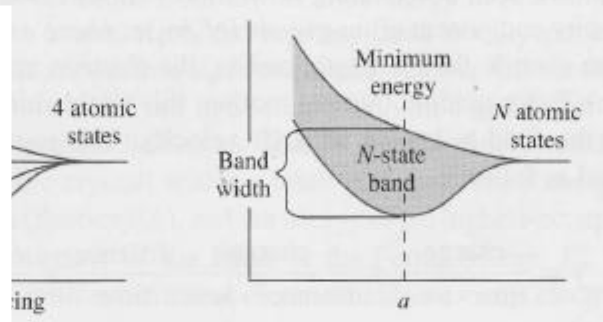
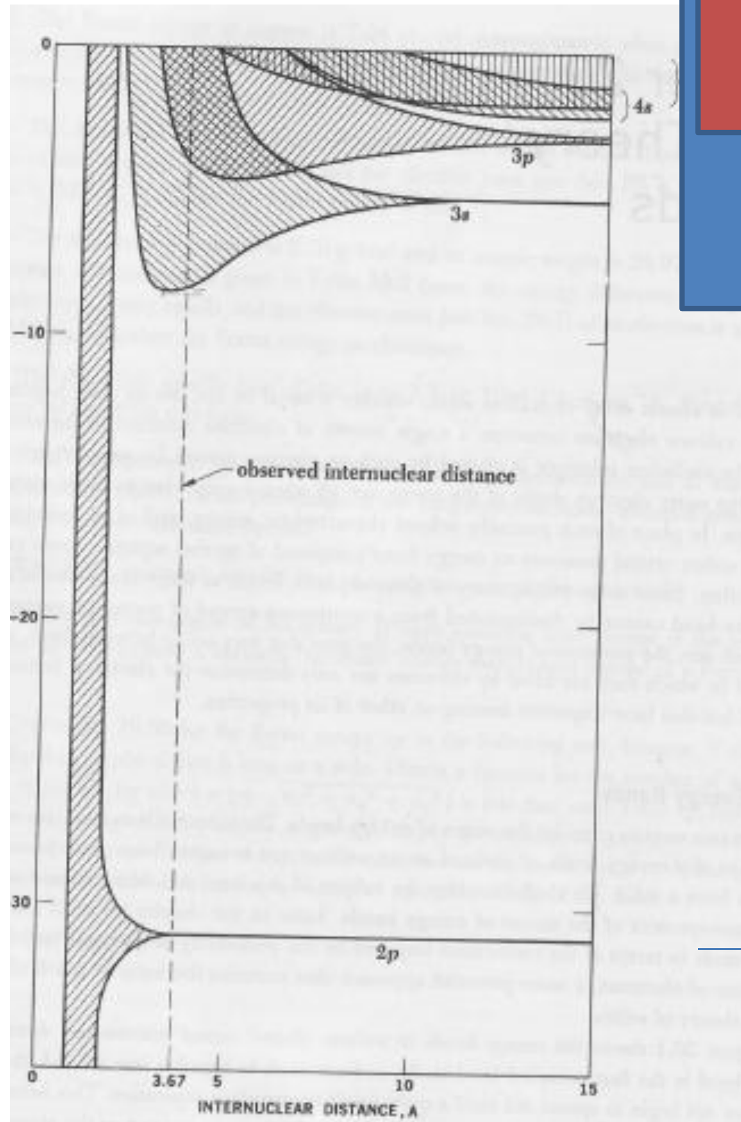


Figure 10.26 Behavior of allowed electron states as atomic spacing varies.

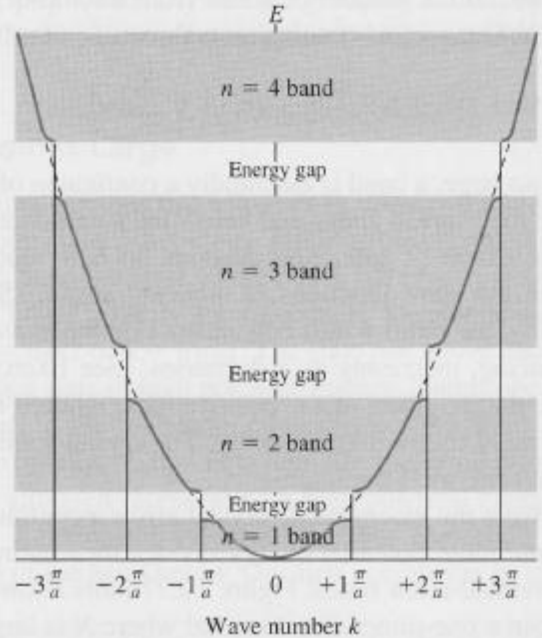




0
−10
−20
30
4s
3p
3s
2p
observed internuclear distance
0
3.67
5
10
15
INTERNUCLEAR DISTANCE, A

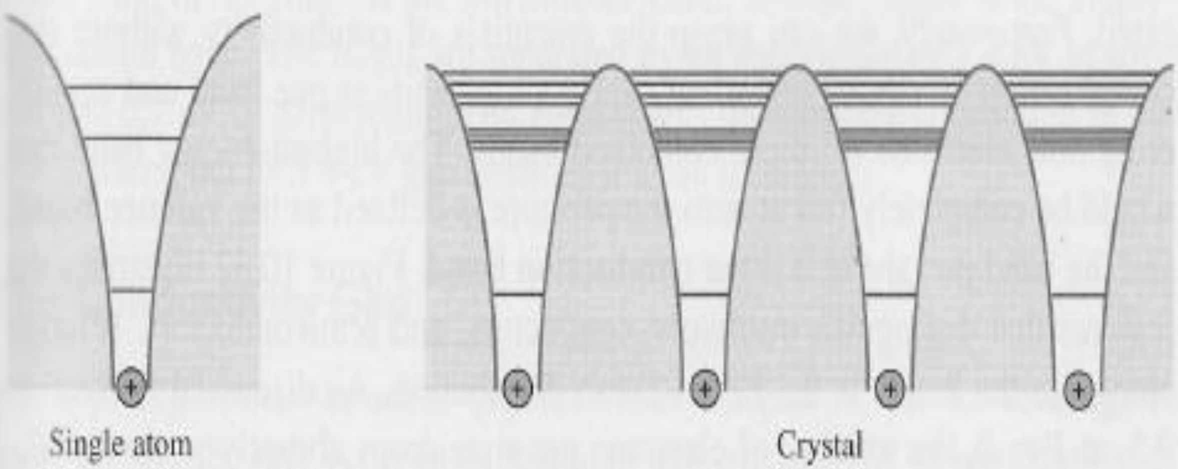
Energy band gap

Figure 10.27 Bands and gaps in a one-dimensional crystal.



Conductors, Insulators, and Semiconductors

Figure 10.29 When atoms form a crystal, low-lying nonvalance levels still belong to each atom, while higher levels become bands.



Band structure

Conductors, Insulators, and Semiconductors

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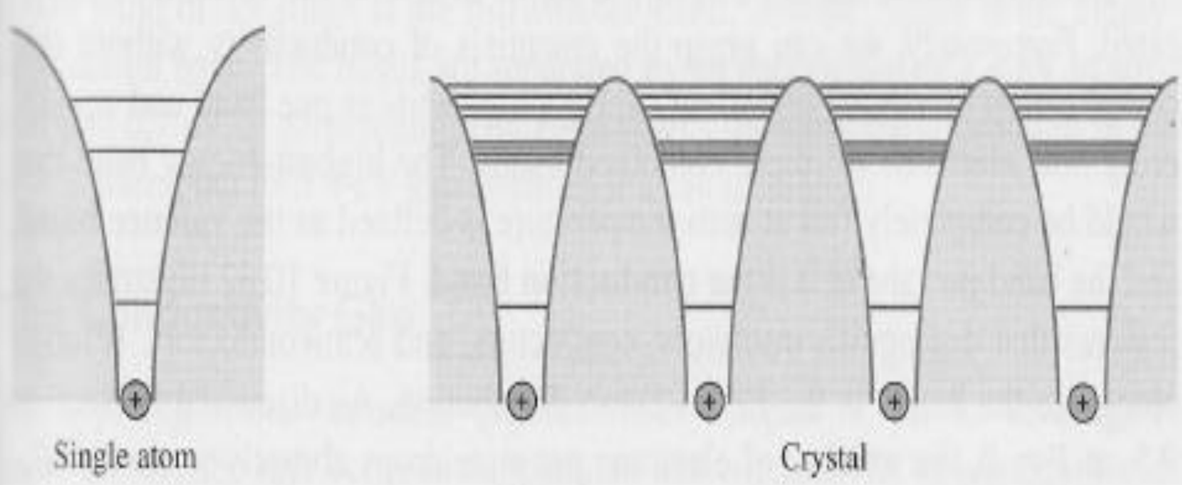


Band structure

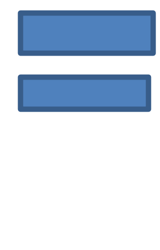
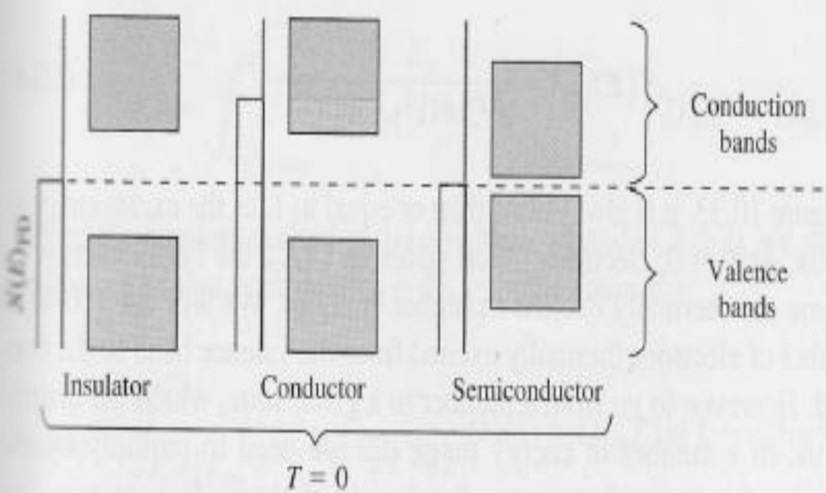


Figure 10.32 Band filling for an insulator, a conductor, and a semiconductor at zero and nonzero temperature. When $T > 0$, a semiconductor will have some electrons in the conduction band.



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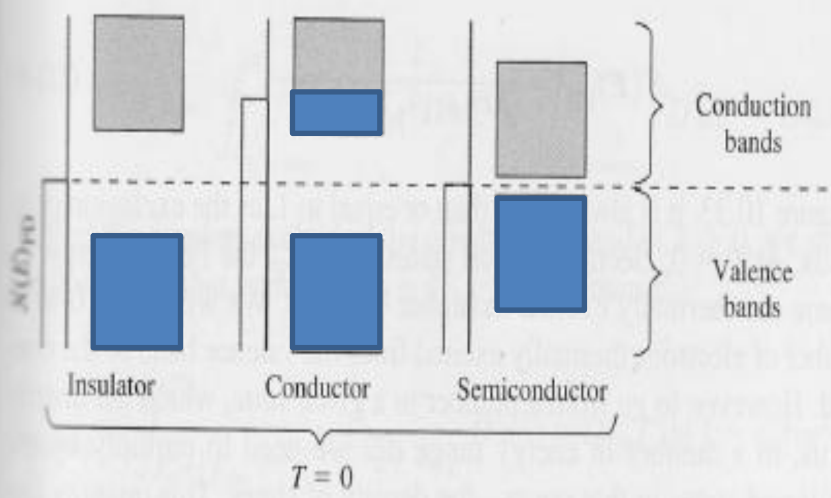
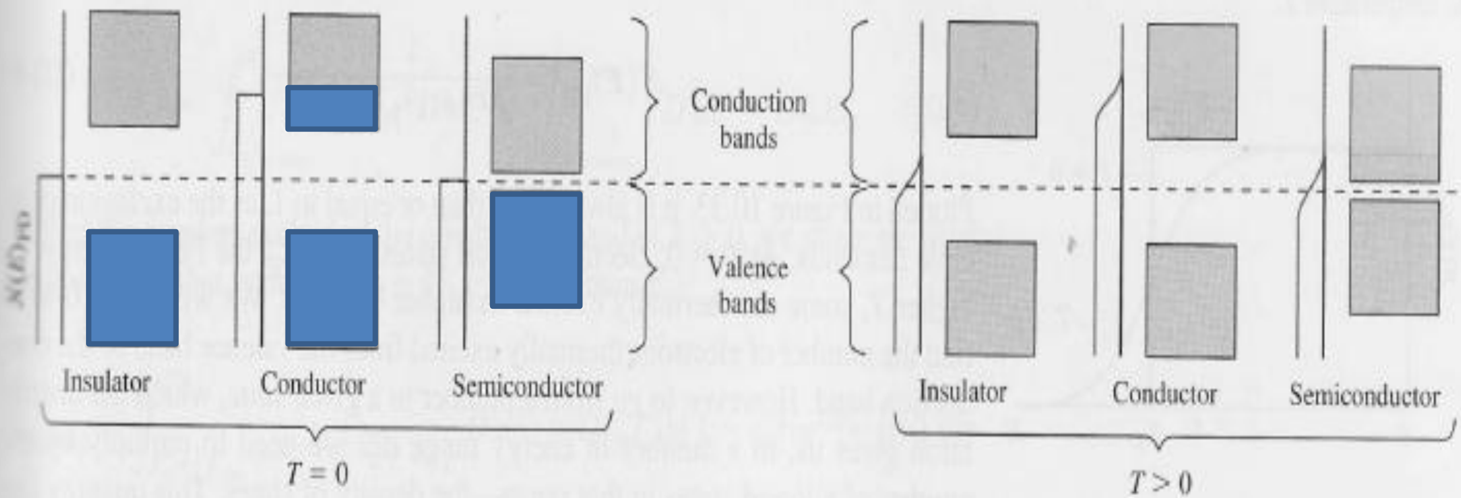


Valence band: The band that is completely filled at T= 0 K
Conduction band: The band that is just above the valence band

Figure 10.32 Band filling for an insulator, a conductor, and a semiconductor at zero and nonzero temperature. When $T > 0$, a semiconductor will have some electrons in the conduction band.



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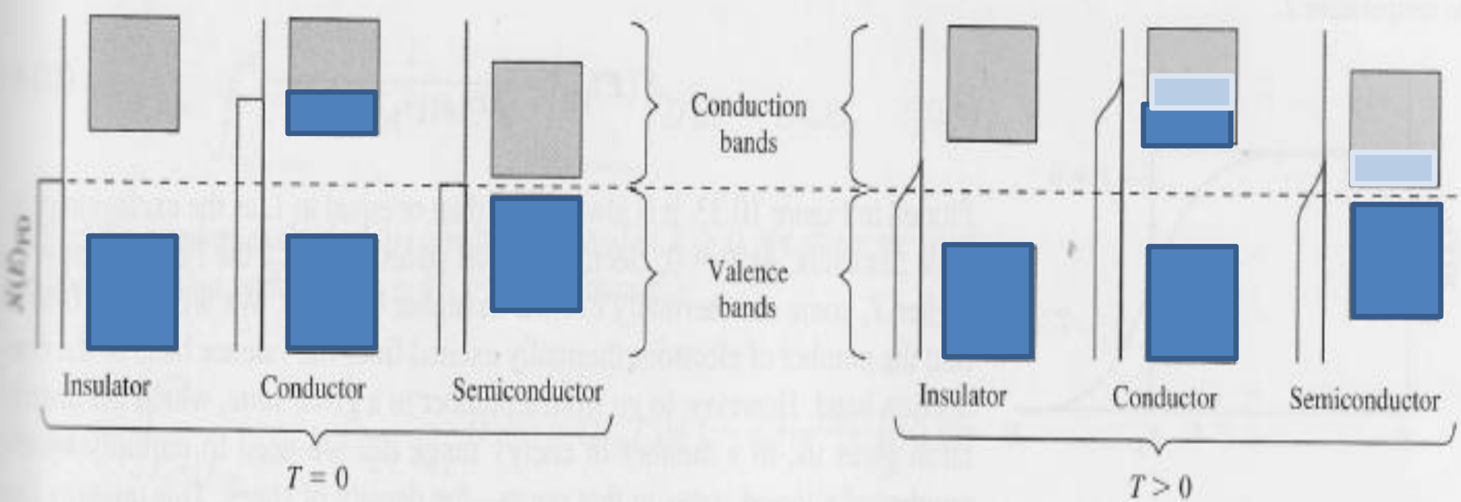
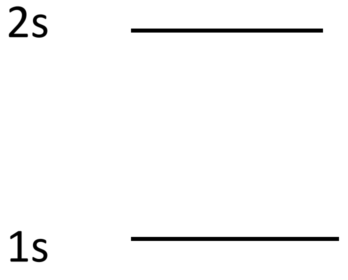


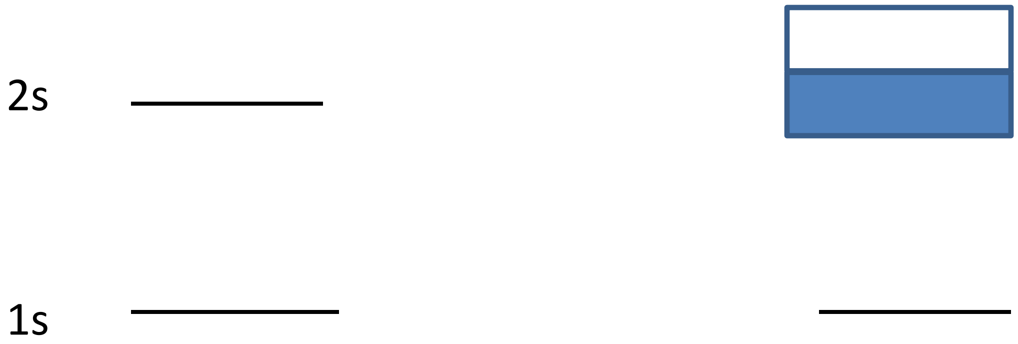
Lithium (Li)



Single Li Atom Energy Levels

Li Solid Energy Levels

Lithium (Li): $1s_2 2s_1$

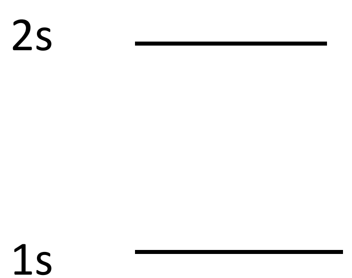


Single Li Atom Energy Levels

Li Solid Energy Levels

Conductor

Beryllium (Be): $1s_2 2s_2$



Single Be Atom Energy Levels

Be Solid Energy Levels

Conductor

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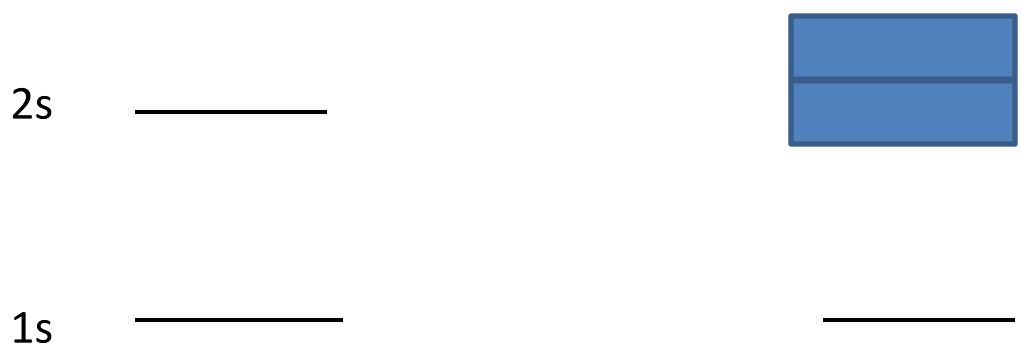

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Be Solid Energy Levels

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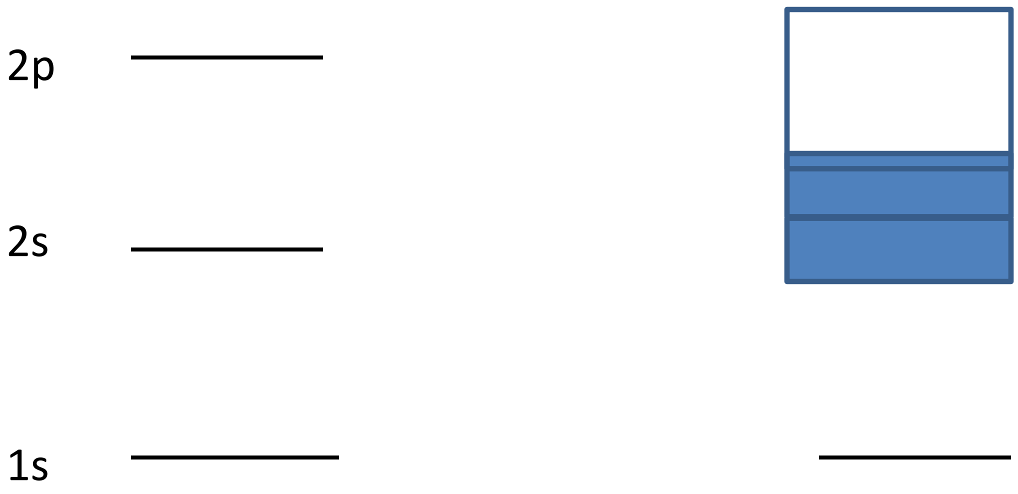

Single Be Atom Energy Levels

Be Solid Energy Levels

Conductor

Conduction

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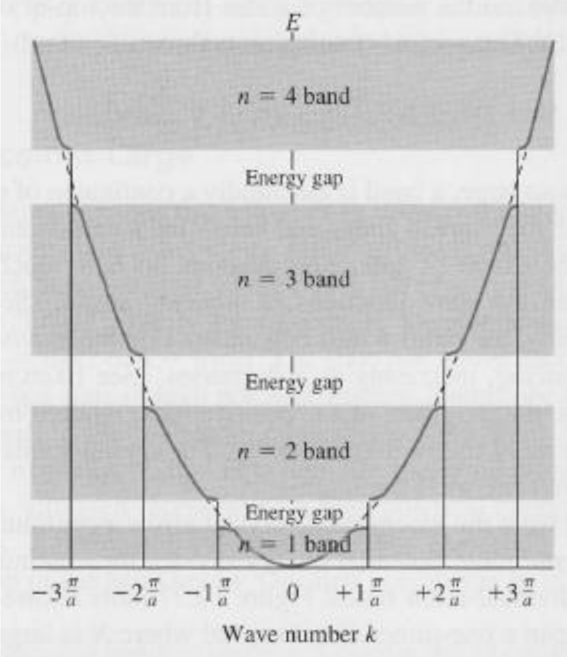
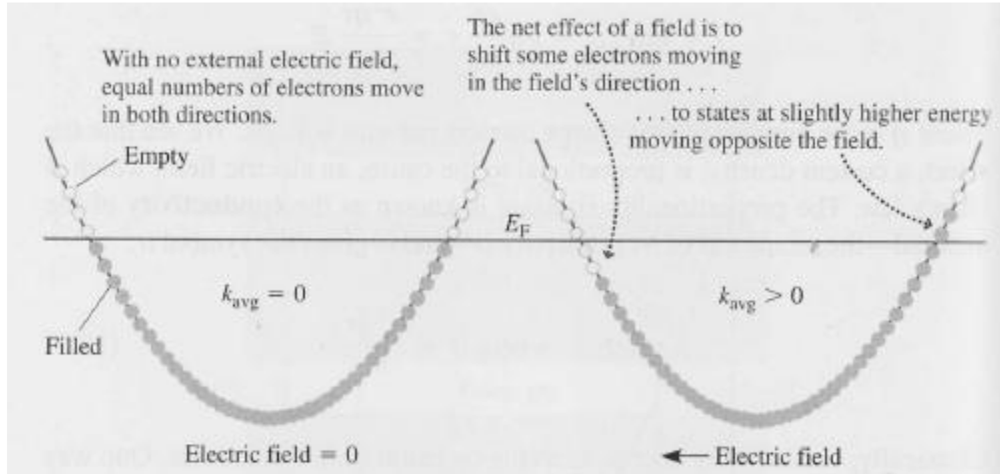
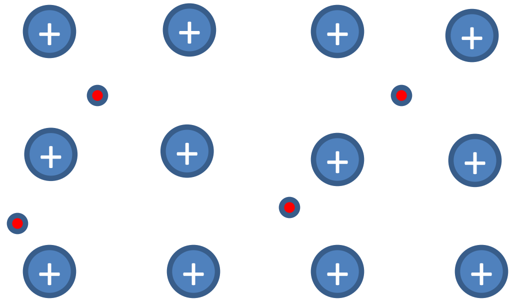


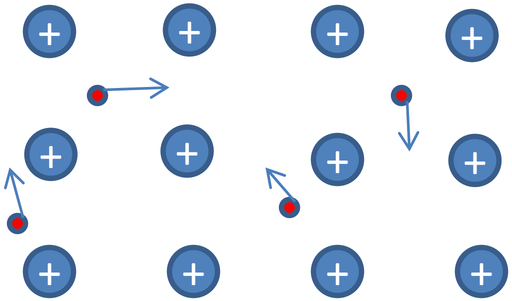


Drift Velocity

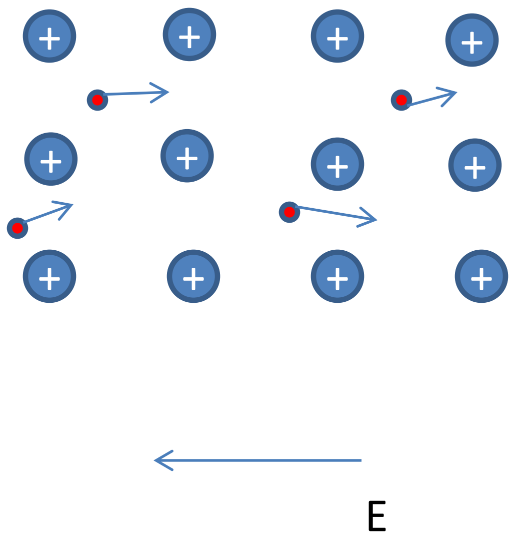


Drift Velocity

No electric field: No net velocity among free electrons



Drift Velocity



Yes electric field: Net velocity (=drift velocity) will emerge.

$$v_{drift} = \frac{eE}{m_e}\tau$$

Drift Velocity

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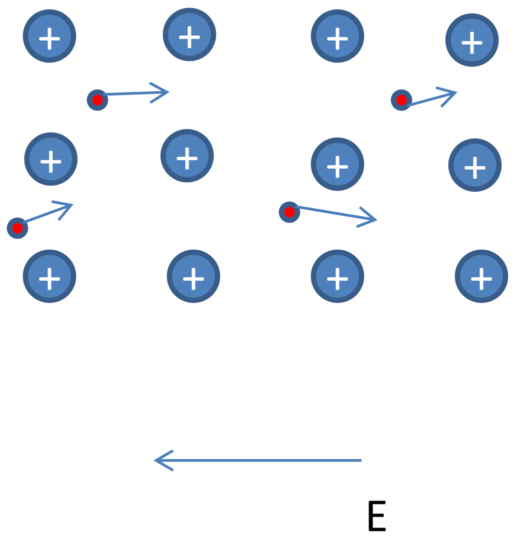

$$v_{drift} = \frac{eE}{m_e}\tau$$

Current density (j)

$$j \equiv \frac{charge}{time \text{ x } area} = \frac{charge}{distance \text{ x } area}\,\frac{distance}{time}$$

$$= \frac{e \text{ x } No.of\ electrons}{volume} v_{drift} = eNv_{drift}$$

$$j = eN\frac{eE}{m_e}\tau = e^2\frac{N\tau}{m_e}E$$

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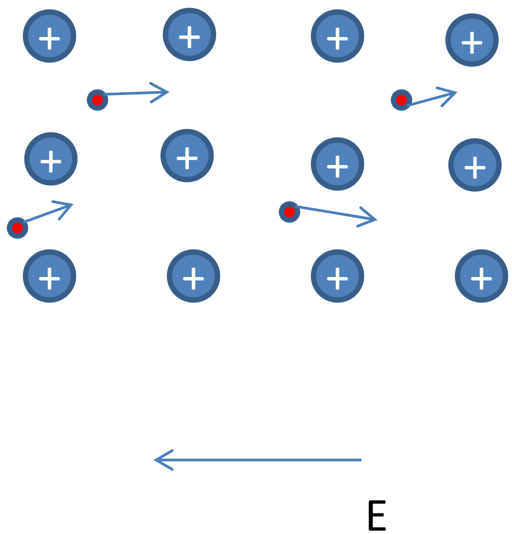

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Conductivity

Silver Example

Density of Silver: $10.5 \text{ x } 10^3 \; kg/m^3$

$$density = \frac{mass\ (= N \text{ x } mass\ of\ one\ Silver\ atom)}{volume\ (= a^3)}$$

$$a = \left(\frac{N \text{ x } mass\ of\ one\ Silver\ atom}{density}\right)^{\frac{1}{3}} = 2.57 \text{ x } 10^{-10}\ m$$

Velocity of electrons associated with E_F

Fermi energy in silver = 5.5 eV

$$E_F = \frac{1}{2} m v^2$$

$$v = \sqrt{\frac{2E_F}{m}} = 1.39\ x\ 10^6\ m/s$$

Collision time

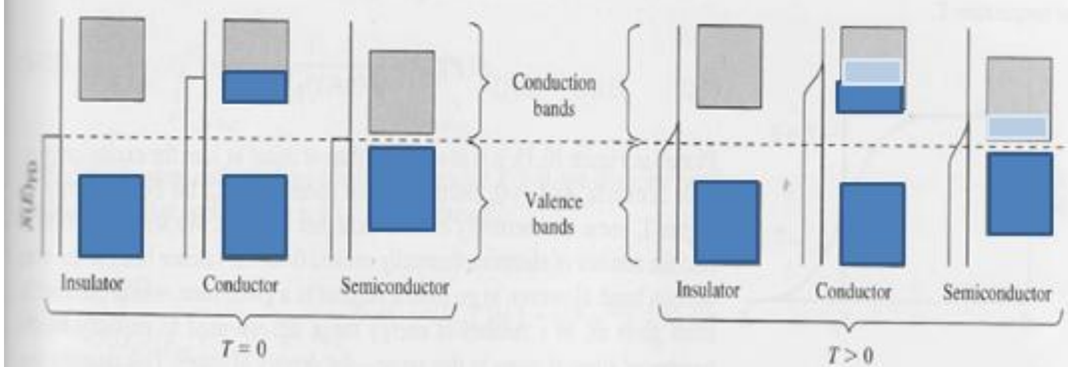
$$\tau = \frac{a}{v} = 1.85 \text{ x } 10^{-16}\ sec$$

Conductivity

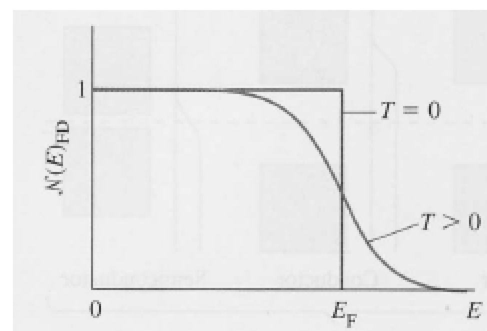
$$\sigma = e^2 \frac{N\tau}{m_e} = 3\ x\ 10^5\ \Omega^{-1} m^{-1}$$

This is much smaller!

Figure 10.32 Band filling for an insulator, a conductor, and a semiconductor at zero and nonzero temperature. When $T > 0$, a semiconductor will have some electrons in the conduction band.



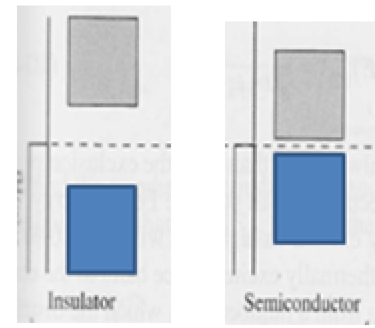
$$\mathcal{N}(E) = \frac{1}{e^{(E-E_F)/k_B T} + 1}$$



$$\mathcal{N}(E) = \frac{1}{e^{(E-E_F)/k_B T} + 1} \qquad D(E) = \mathrm{D}$$

$$N_{Valence} = \int_{E_{valence-bottom}}^{E_{valence-top}} \mathcal{N}(E) D(E) dE$$

$$= \int_{E_{valence-bottom}}^{E_{valence-top}} 1 \cdot D dE = D \Delta E_{Valence}$$



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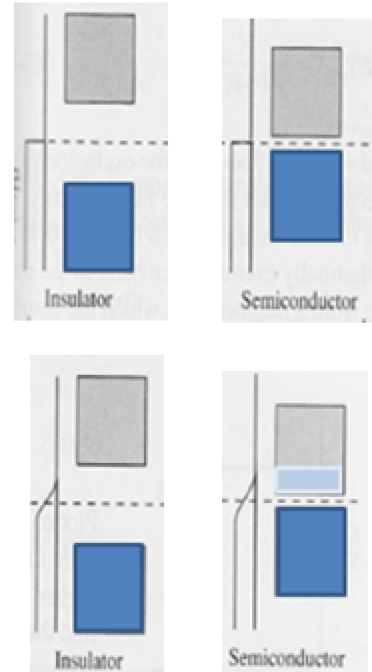

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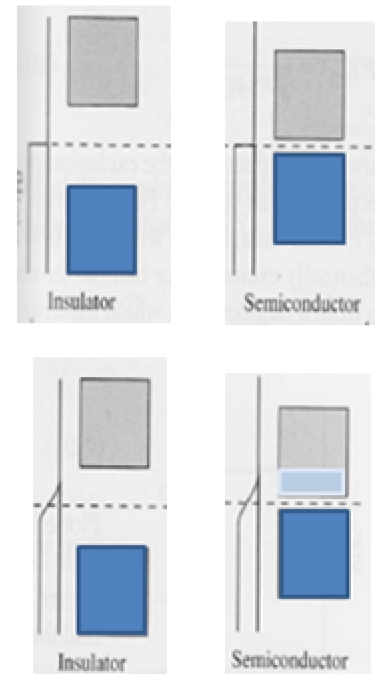
$$N_{Excited} = \int_{E_F + \frac{1}{2}E_{gap}}^{\infty} \mathcal{N}(E) D(E) dE$$

$$= \int_{E_F + \frac{1}{2}E_{gap}}^{\infty} \frac{D}{e^{(E-E_F)/k_B T} + 1} dE = D k_B T \ln(1 + e^{-E_{gap}/2k_B T}) \sim D k_B T e^{-E_{gap}/2k_B T}$$

$\ln(1+x) \sim x$ *when* x *is small*

$$\mathcal{N}(E) = \frac{1}{e^{(E-E_F)/k_BT} + 1} \qquad D(E) = \mathrm{D}$$



$$N_{Valence} = \int_{E_{valence-bottom}}^{E_{valence-top}} \mathcal{N}(E) D(E) dE$$

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$$\frac{N_{Excited}}{N_{Valence}} = \frac{D k_B T e^{-E_{gap}/2k_BT}}{D\Delta E_{Valence}} = \frac{k_B T}{\Delta E_{Valence}} e^{-E_{gap}/2k_BT}$$

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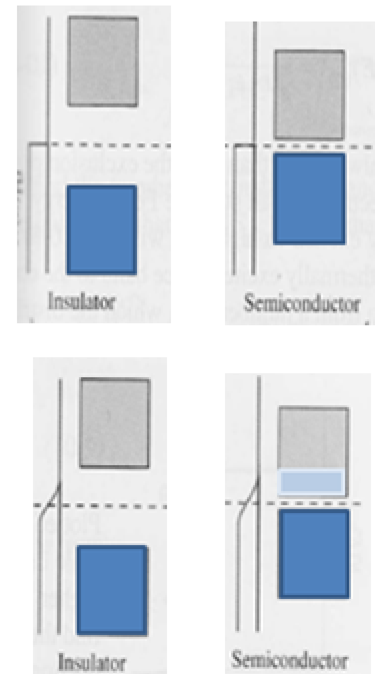
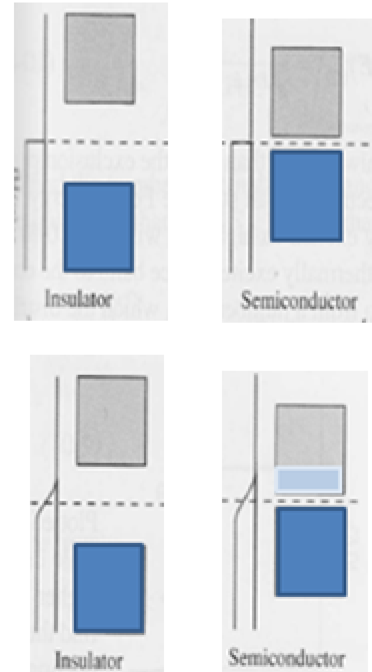


$$\frac{N_{Excited}}{N_{Valence}} = \frac{D k_B T e^{-E_{gap}/2k_B T}}{D \Delta E_{Valence}} = \frac{k_B T}{\Delta E_{Valence}} e^{-E_{gap}/2k_B T}$$

0.0026 eV

$$\mathcal{N}(E) = \frac{1}{e^{(E-E_F)/k_BT} + 1} \qquad D(E) = \mathrm{D}$$



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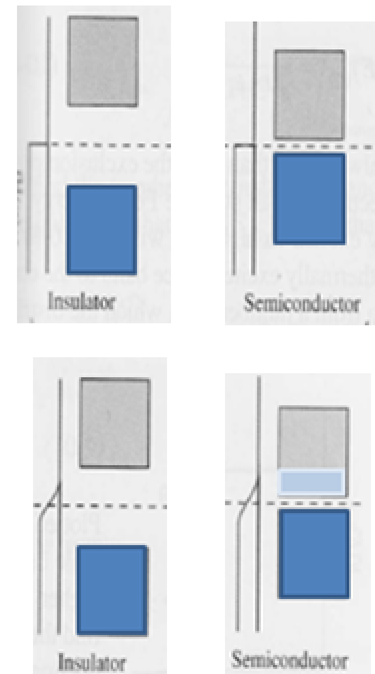
$$\frac{N_{Excited}}{N_{Valence}} = \frac{Dk_BTe^{-E_{gap}/2k_BT}}{D\Delta E_{Valence}} = \frac{k_BT}{\Delta E_{Valence}} e^{-E_{gap}/2k_BT}$$

Insulator band gap: 5 eV

Semiconductor band gap: 1 eV

Energy band size~10 eV, k_BT at 300K = 0.026eV

$$\mathcal{N}(E) = \frac{1}{e^{(E-E_F)/k_BT}+1} \qquad D(E) = \mathrm{D}$$



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Insulator band gap: 5 eV

$\sim 10^{-42}$

Semiconductor band gap: 1 eV

$\sim 10^{-8}$

Energy band size~10 eV, k_BT at 300K = 0.026eV