

# Electrons in Crystals

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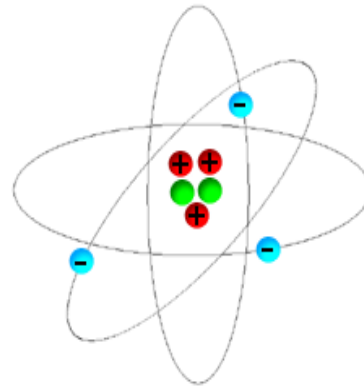
# Electrons

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Charge =  $-1.6022 \times 10^{-19}$  C

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

Radius = ?



0.15 nm

[www.alnaden.ibm.com/vis/stm/atomo.html](http://www.alnaden.ibm.com/vis/stm/atomo.html)

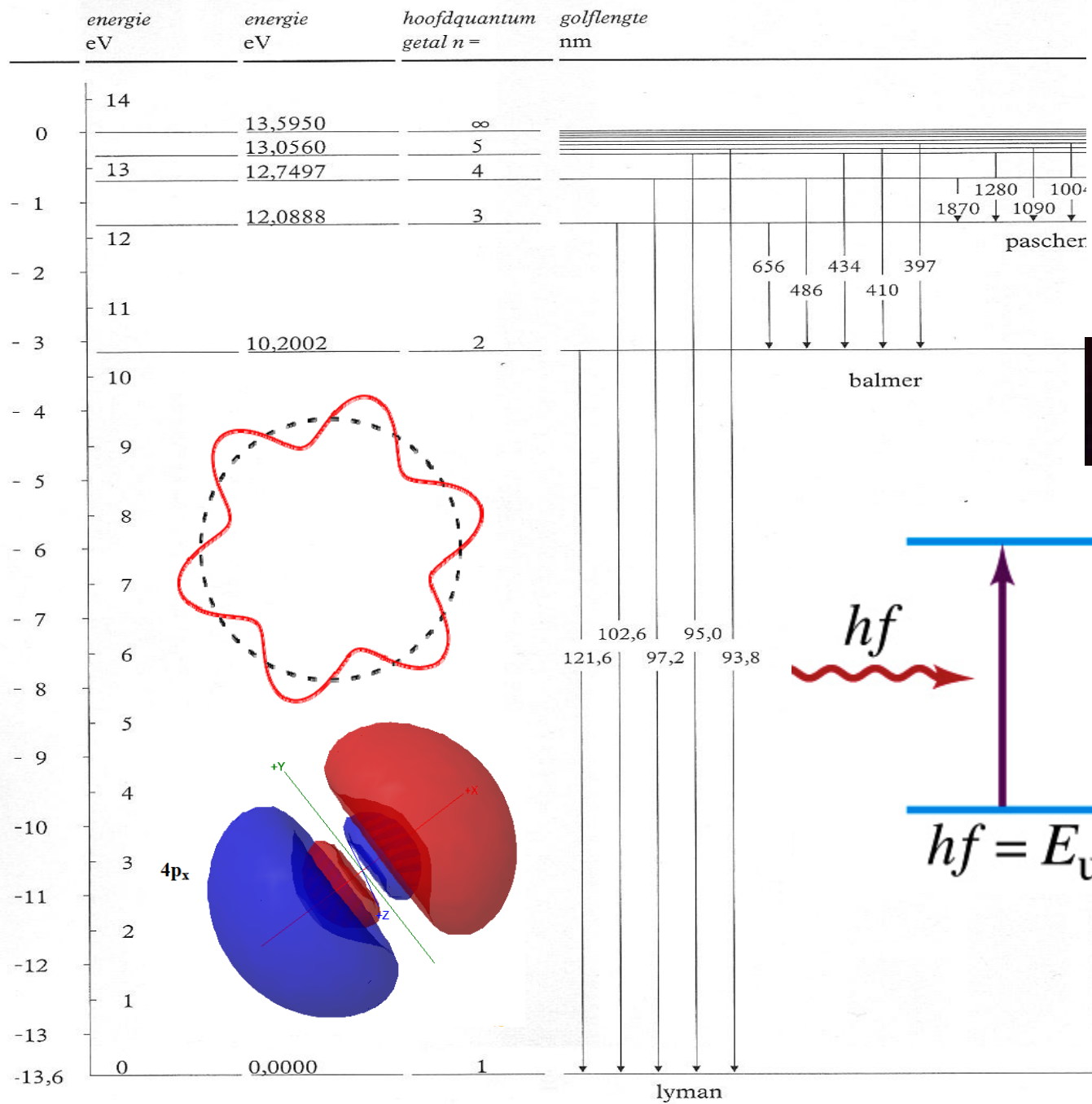
# Quantum Mechanics

Everything moves like a wave but exchanges energy and momentum like a particle.

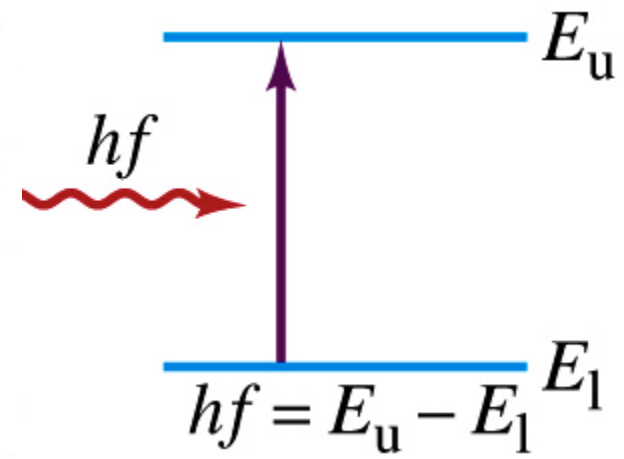
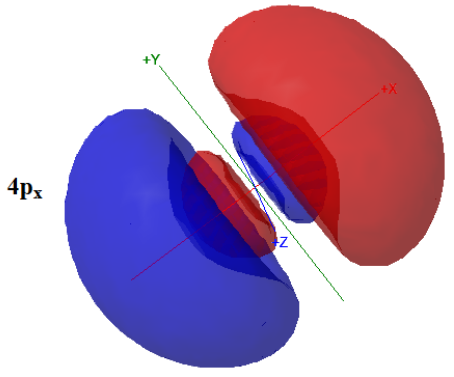
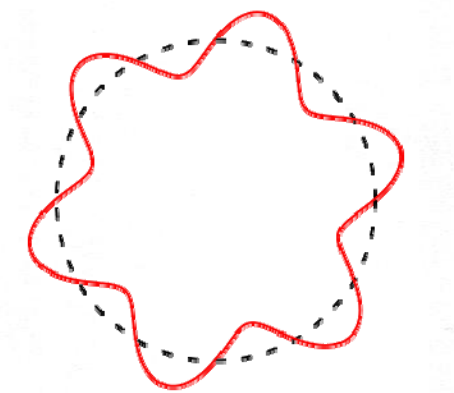
Everything moves like a wave but exchanges energy and momentum like a particle.



de aangegeven golflengten gelden in vacuüm

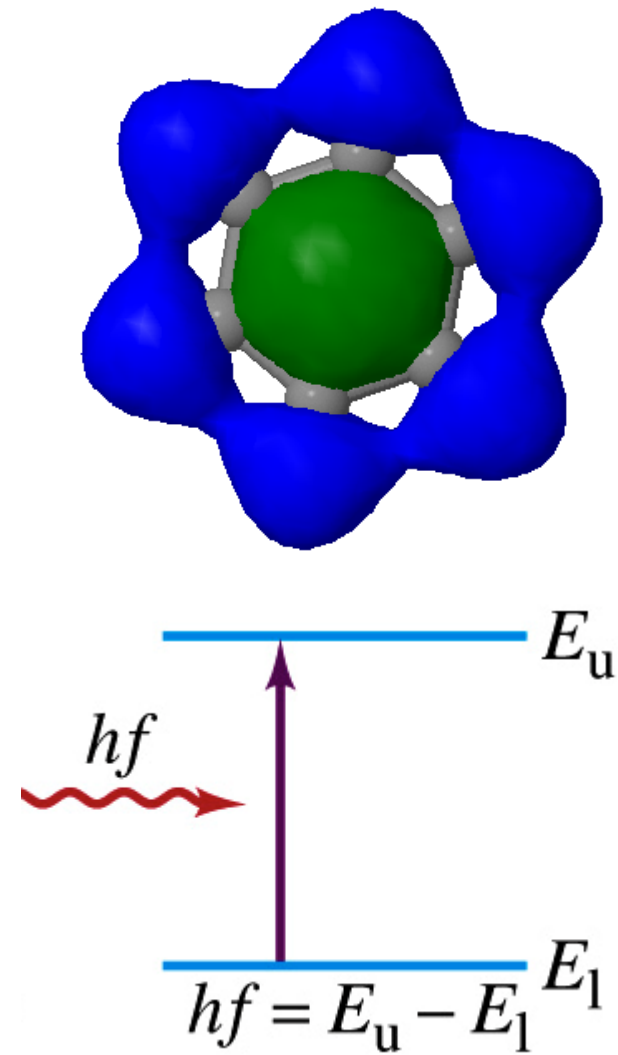
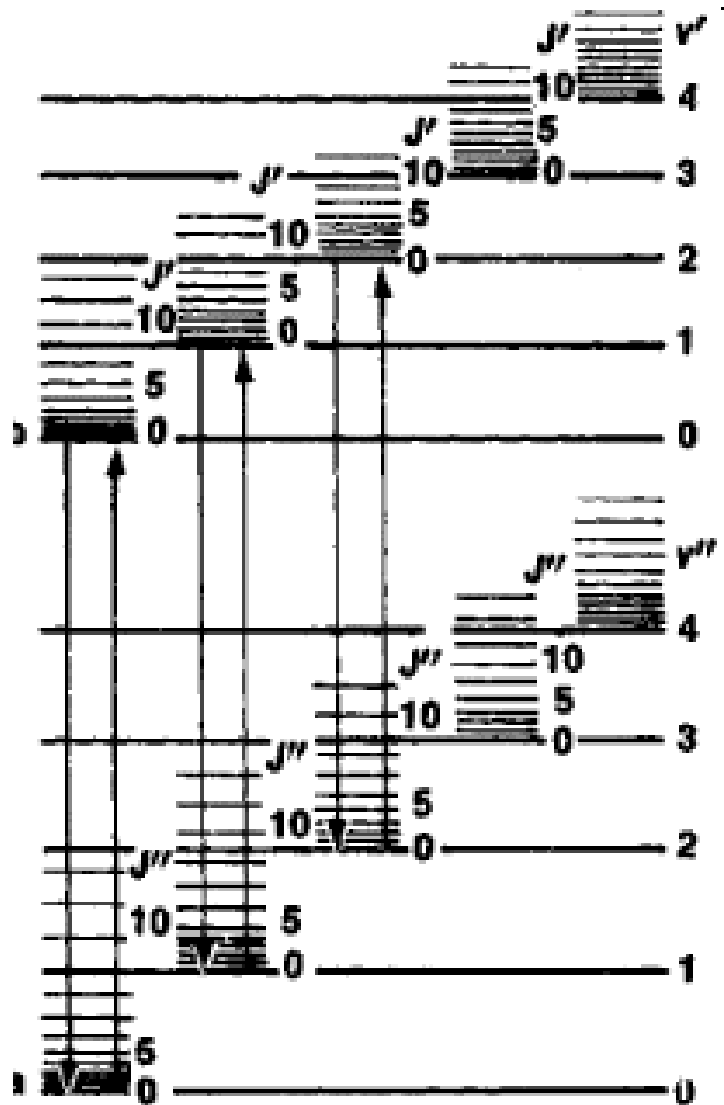


Fluorescent lamp

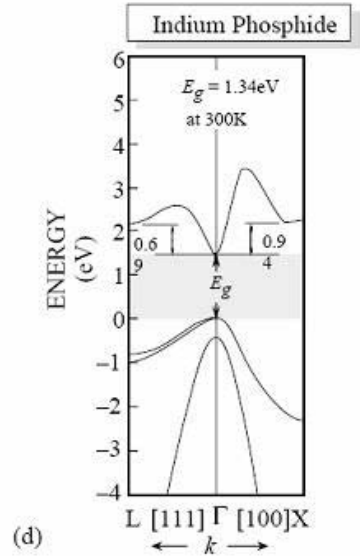
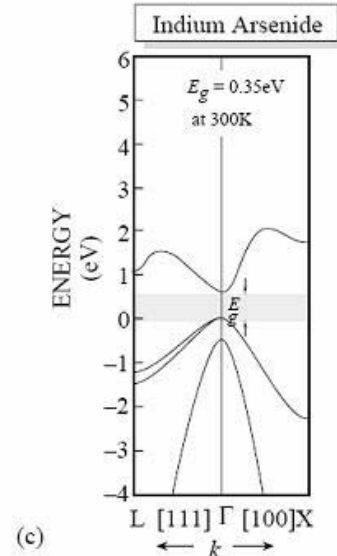
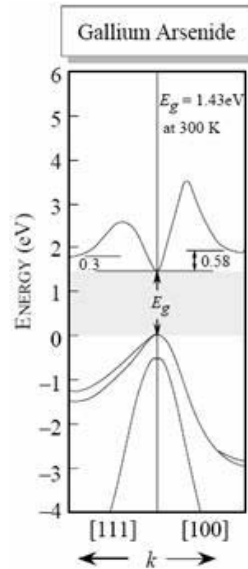
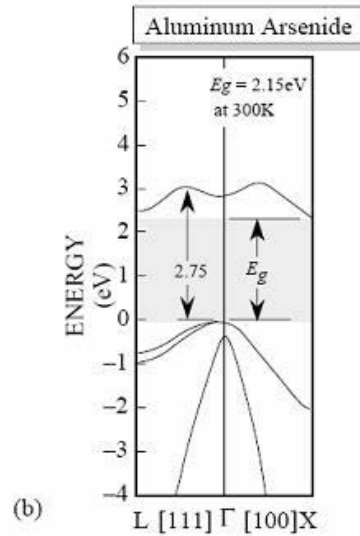
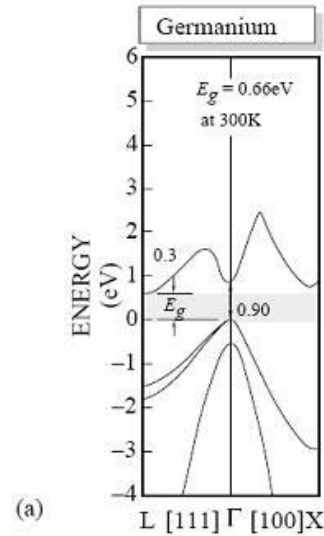
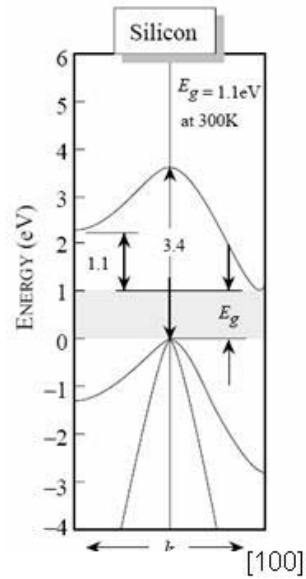


lyman

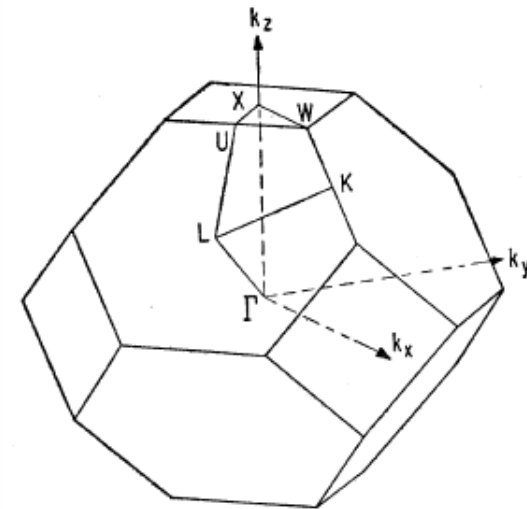
# Molecular energy levels



# Semiconductors



valence band  
 conduction band  
 band gap



molecular orbitals  
 are plane waves

# wave vector $k$

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A  $k$ -vector points in the direction a wave is propagating.

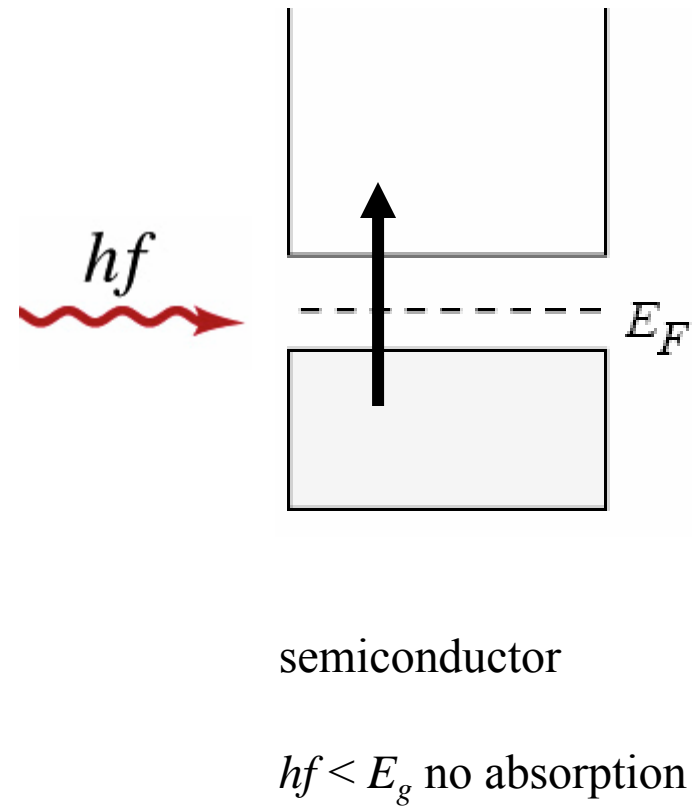
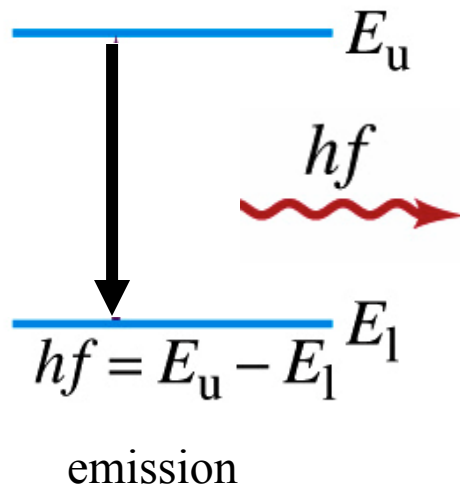
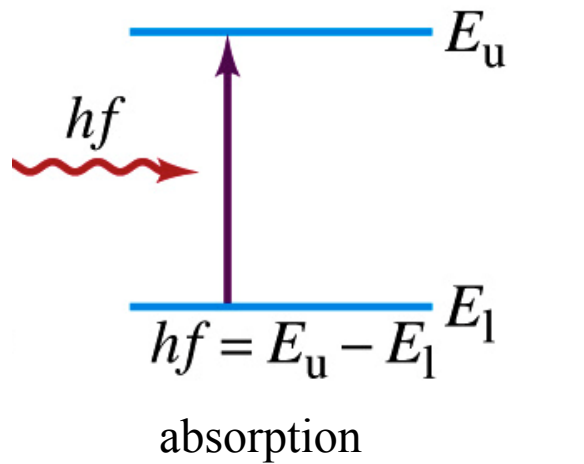
wavelength:  $\lambda = \frac{2\pi}{|\vec{k}|}$

momentum:  $\vec{p} = \hbar\vec{k}$



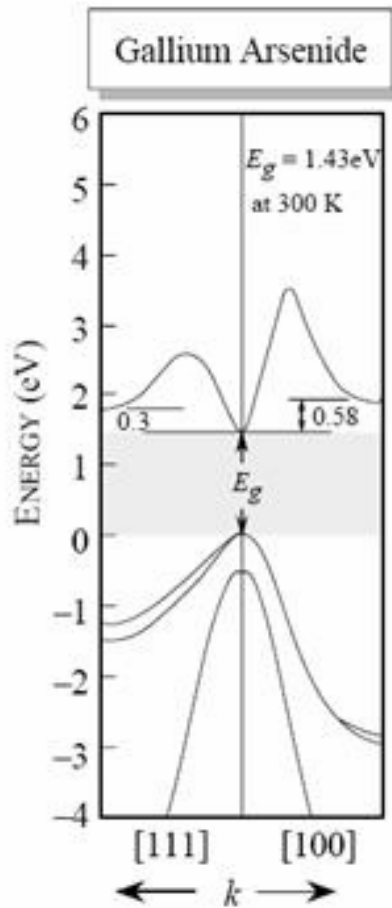
# Absorption and emission of photons

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# What color light does a GaAs LED emit?

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$$E = 1.6022 \times 10^{-19} \times 1.43 \text{ J} = hf = \frac{hc}{\lambda}$$

$$\lambda = 867 \text{ nm} \quad \text{infrared}$$

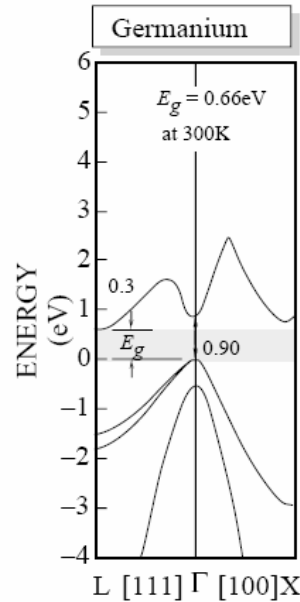
# Direct and indirect band gaps

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indirect bandgap

$$\Delta k \neq 0$$

phonons are emitted

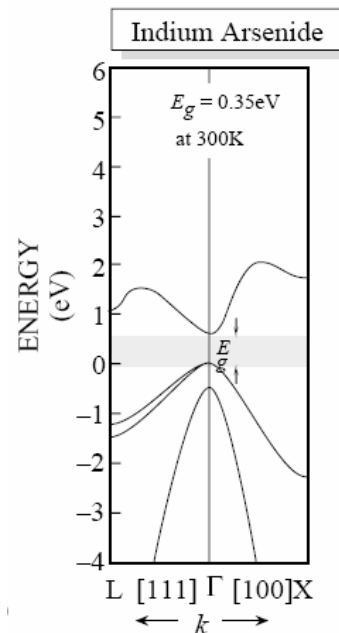


Momentum must be conserved when photons are absorbed or emitted.

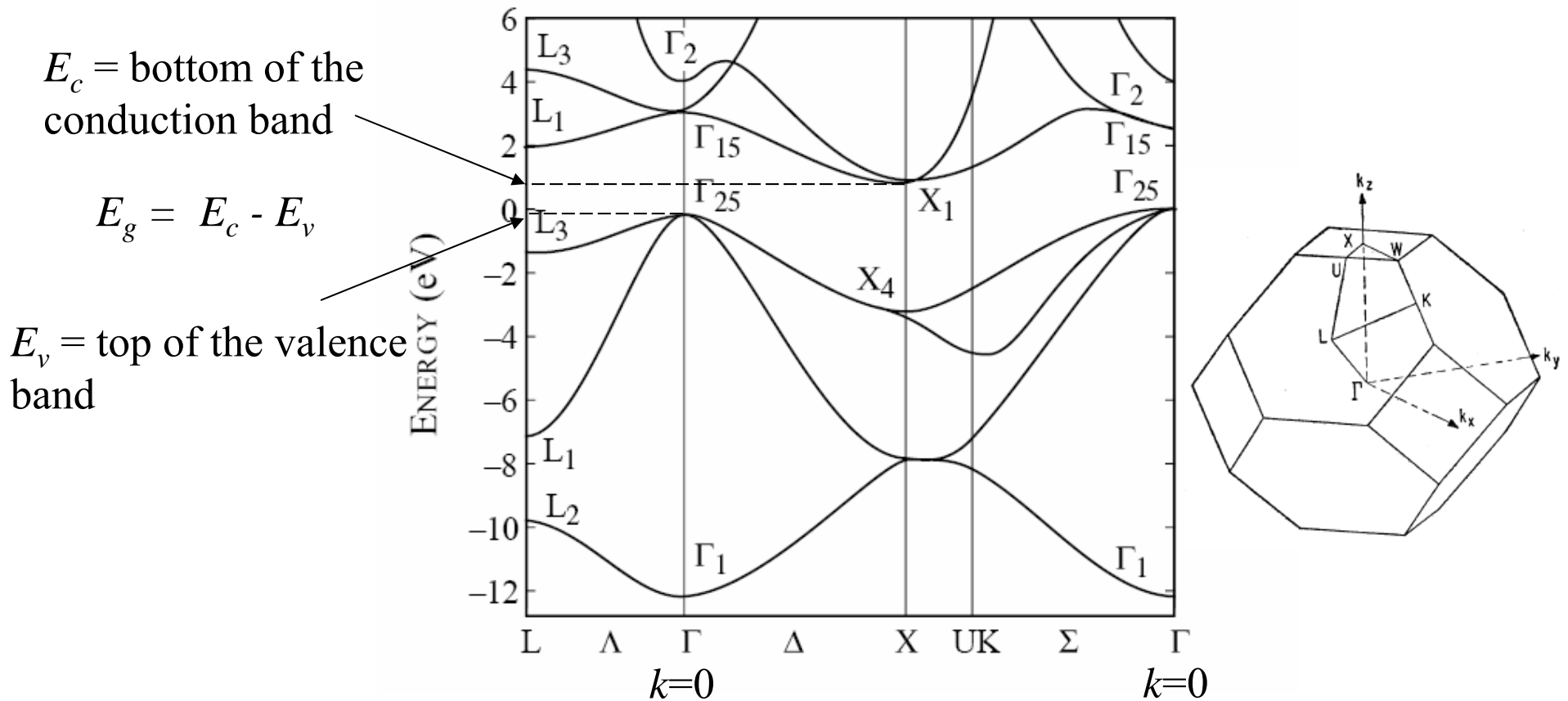
direct bandgap:

$$\Delta k = 0$$

photons can be emitted



# Silicon band structure

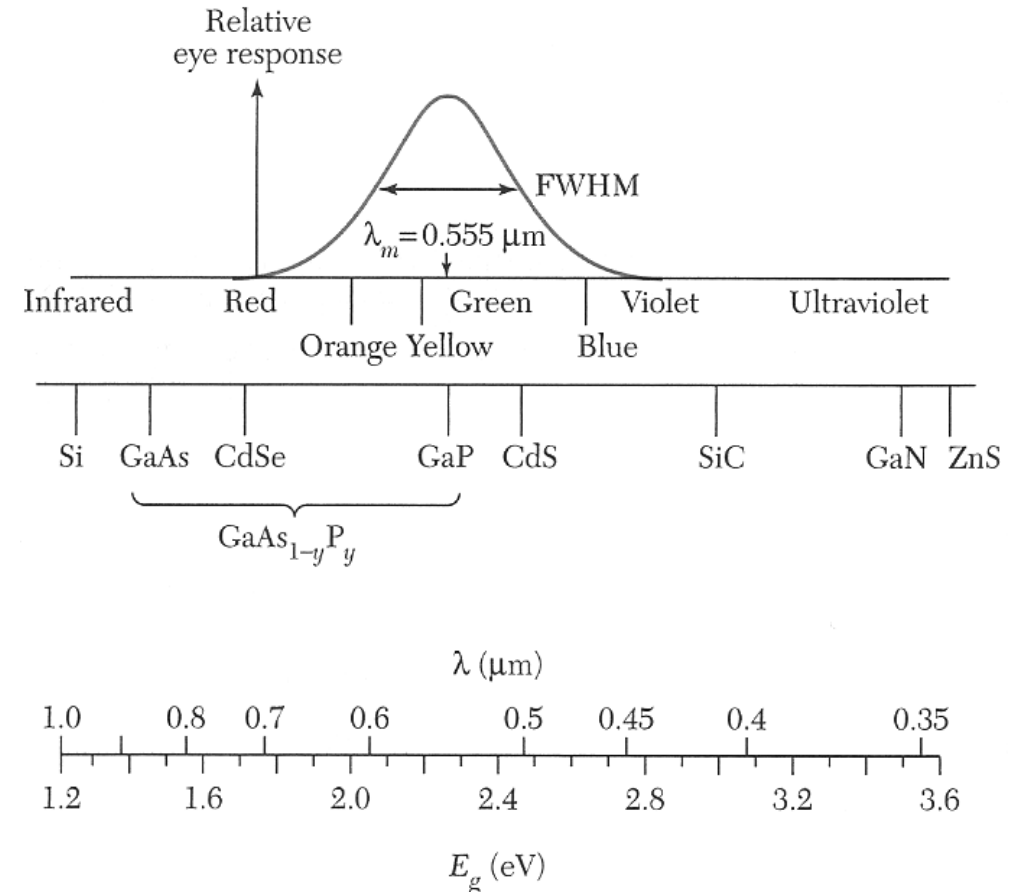


Electrons with energies in the gap are reflected out of the crystal.

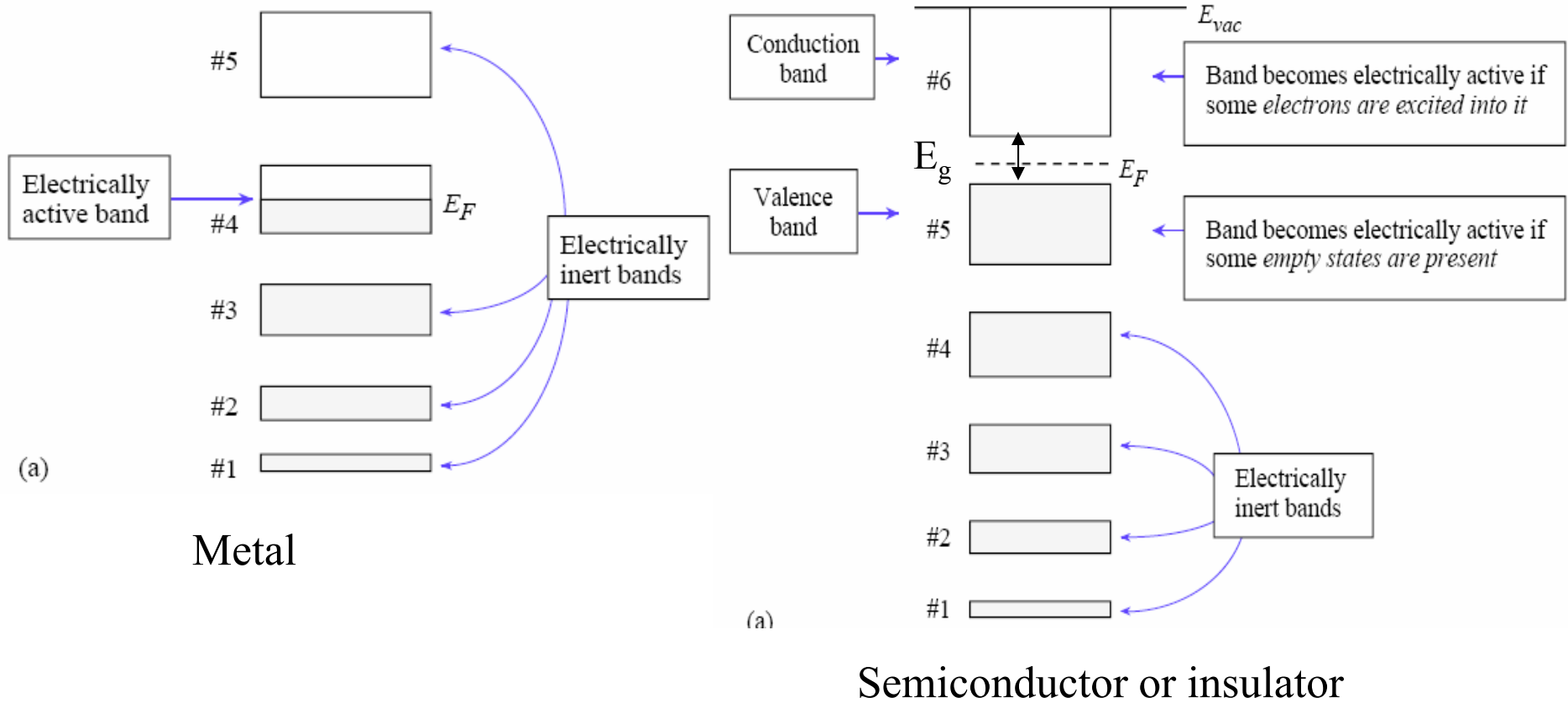
**TABLE 1 Common III-V materials used to produce LEDs and their emission wavelengths.**

Material	Wavelength (nm)
InAsSbP/InAs	4200
InAs	3800
GaInAsP/GaSb	2000
GaSb	1800
$Ga_xIn_{1-x}As_{1-y}P_y$	1100-1600
$Ga_{0.47}In_{0.53}As$	1550
$Ga_{0.27}In_{0.73}As_{0.63}P_{0.37}$	1300
GaAs:Er, InP:Er	1540
Si:C	1300
GaAs:Yb, InP:Yb	1000
$Al_xGa_{1-x}As:Si$	650-940
GaAs:Si	940
$Al_{0.11}Ga_{0.89}As:Si$	830
$Al_{0.4}Ga_{0.6}As:Si$	650
$GaAs_{0.6}P_{0.4}$	660
$GaAs_{0.4}P_{0.6}$	620
$GaAs_{0.15}P_{0.85}$	590
$(Al_xGa_{1-x})_{0.5}In_{0.5}P$	655
GaP	690
GaP:N	550-570
$Ga_xIn_{1-x}N$	340,430,590
SiC	400-460
BN	260,310,490

# Light emitting diodes



# Metals, semiconductors, insulators

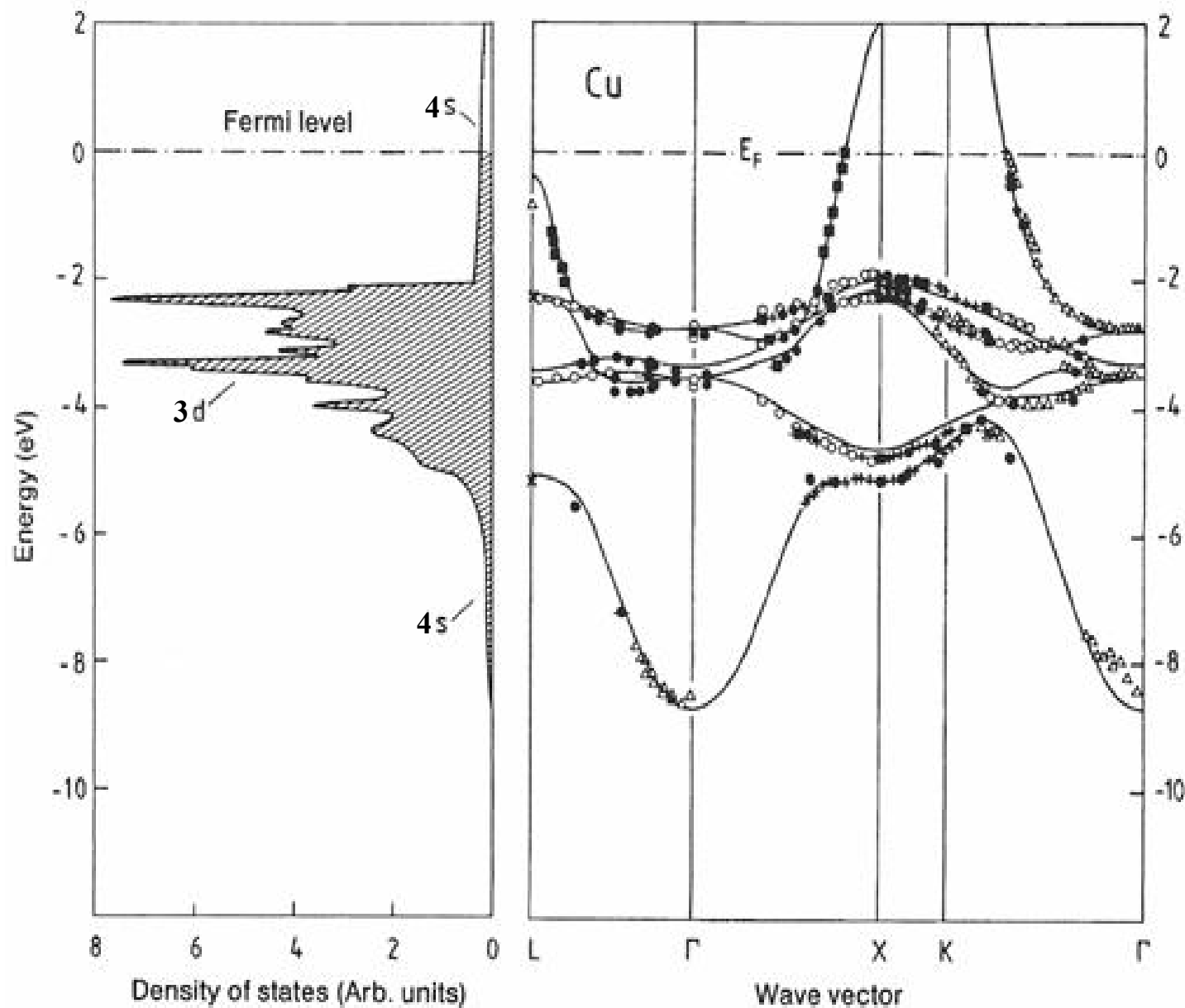


$E_g < 3\text{eV} = \text{Semiconductor}$

$E_g > 3\text{eV} = \text{Insulator}$

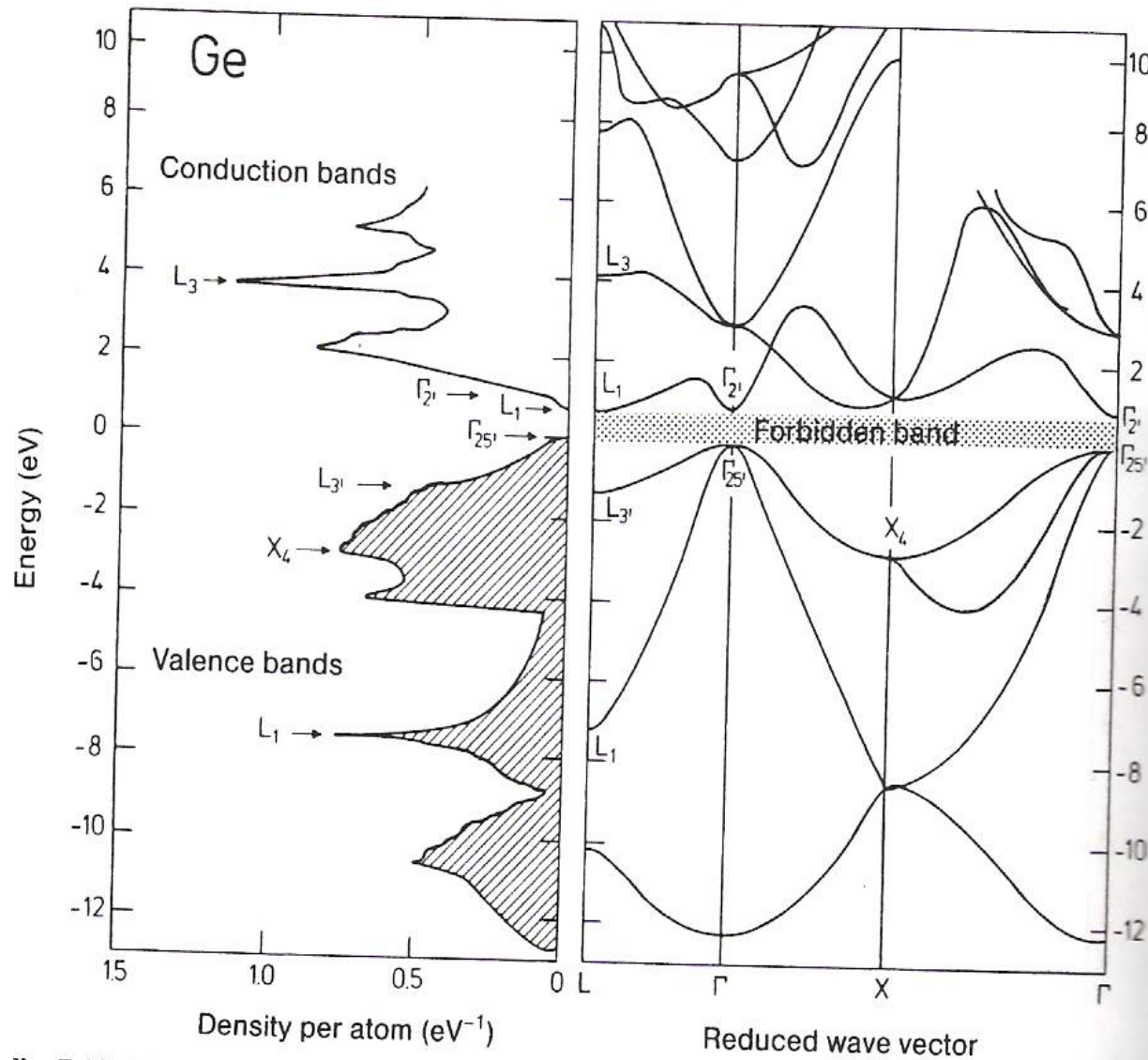
from: Singh

# Copper dispersion relation and density of states



from Ibach & Lueth

# Germanium

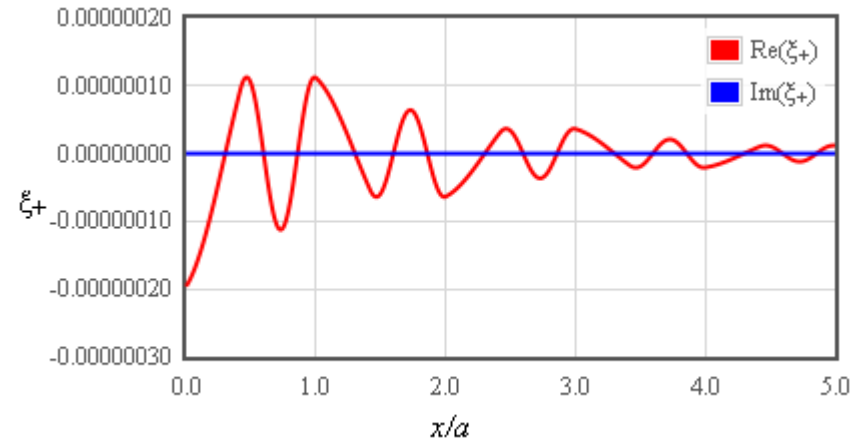
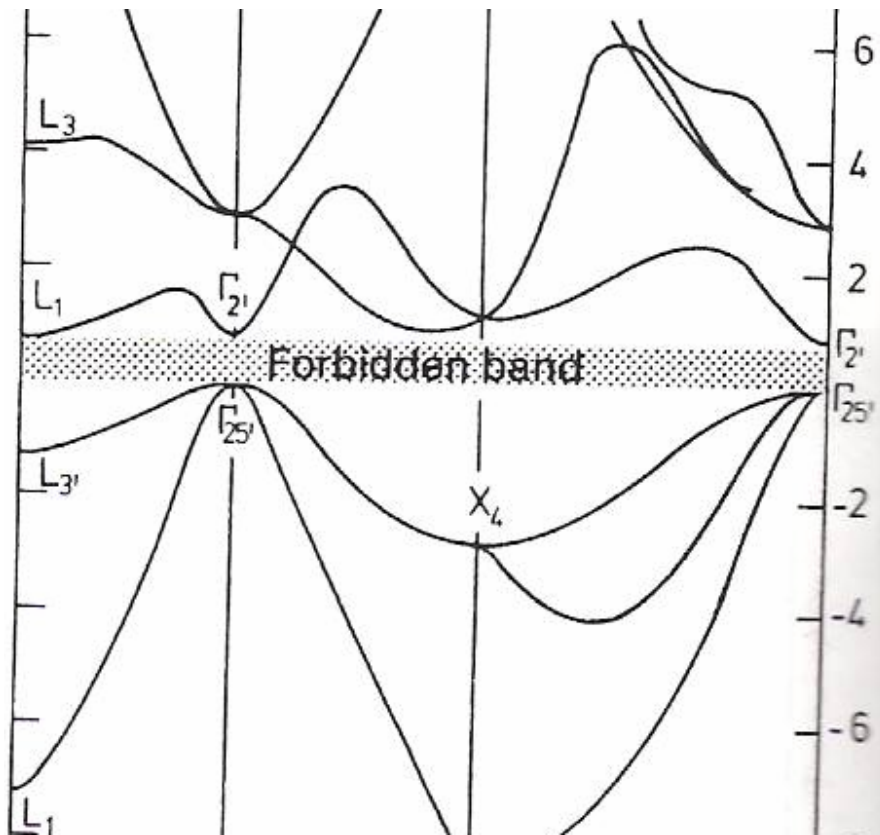


from Ibach & Lueth



# Band gap

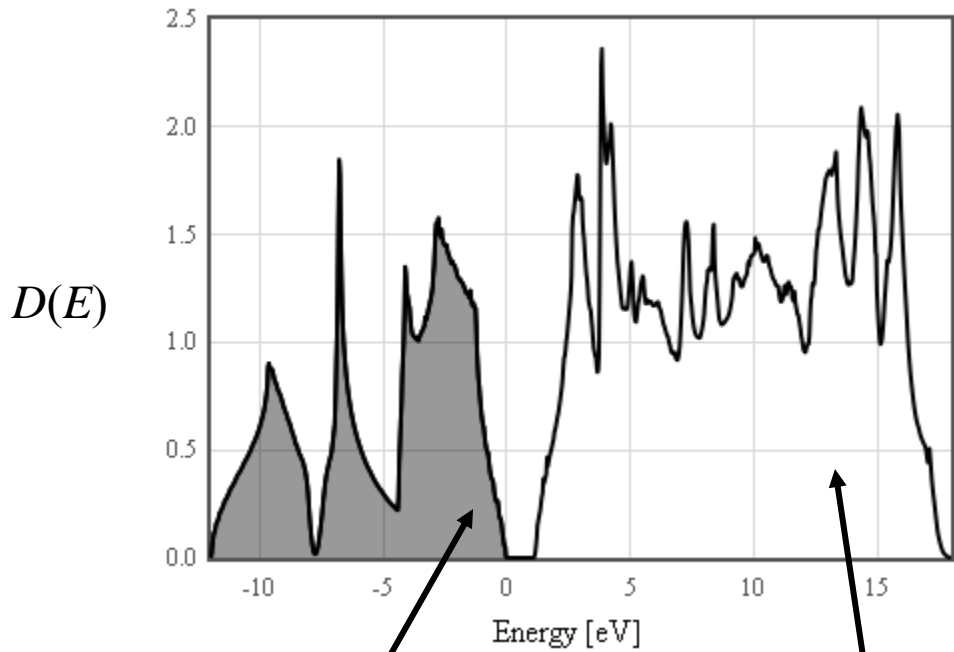
Electrons with energies in the gap are reflected out of the crystal.



# Density of states

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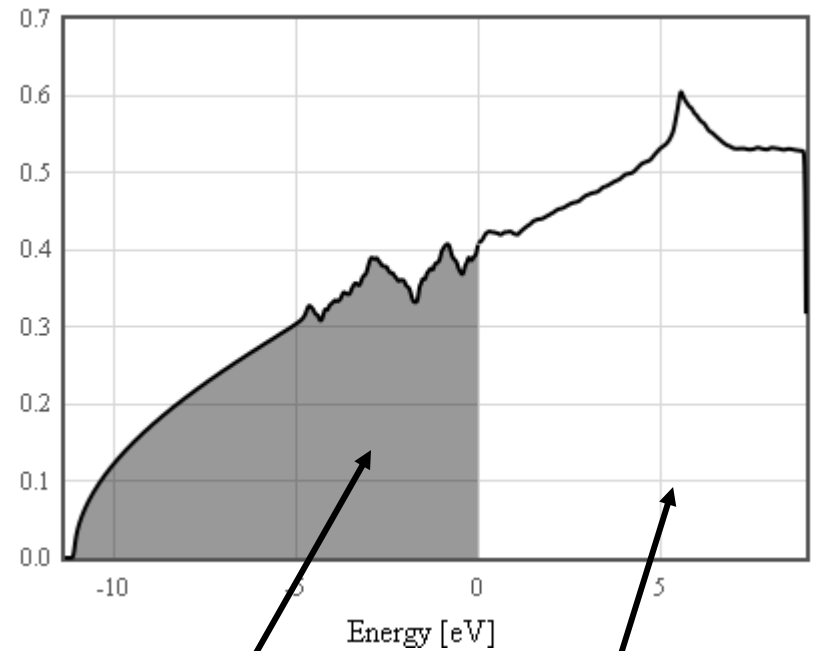
Silicon



filled states

empty states

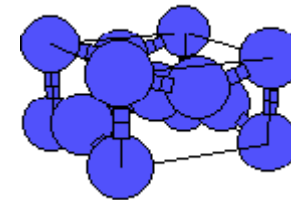
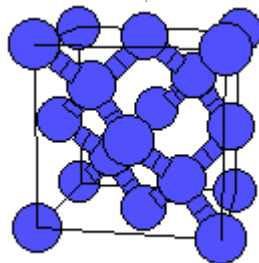
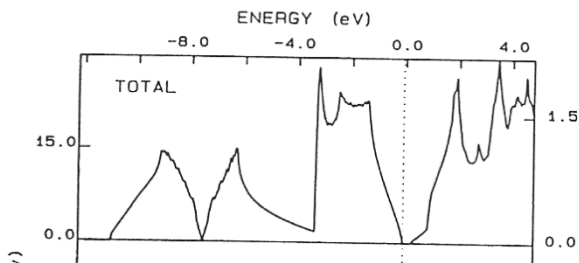
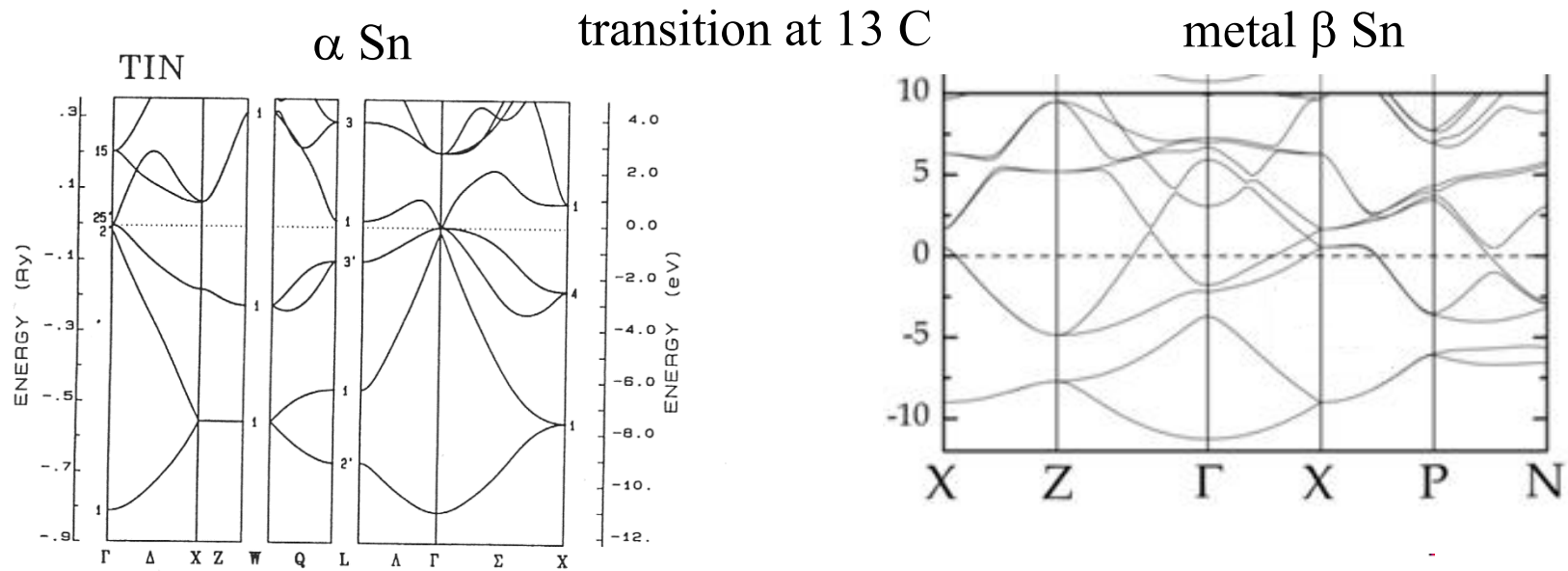
Aluminum



filled states

empty states

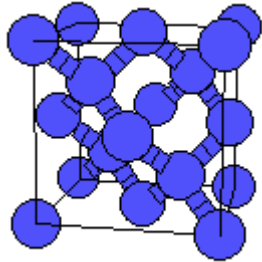
# Structural phase transition in Sn



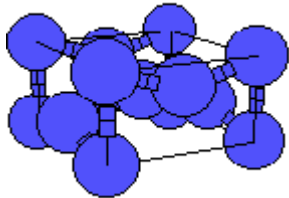
$\beta$ -Sn, white tin, tetragonal

$\alpha$ -Sn, gray tin, diamond structure

# Structural phase transitions

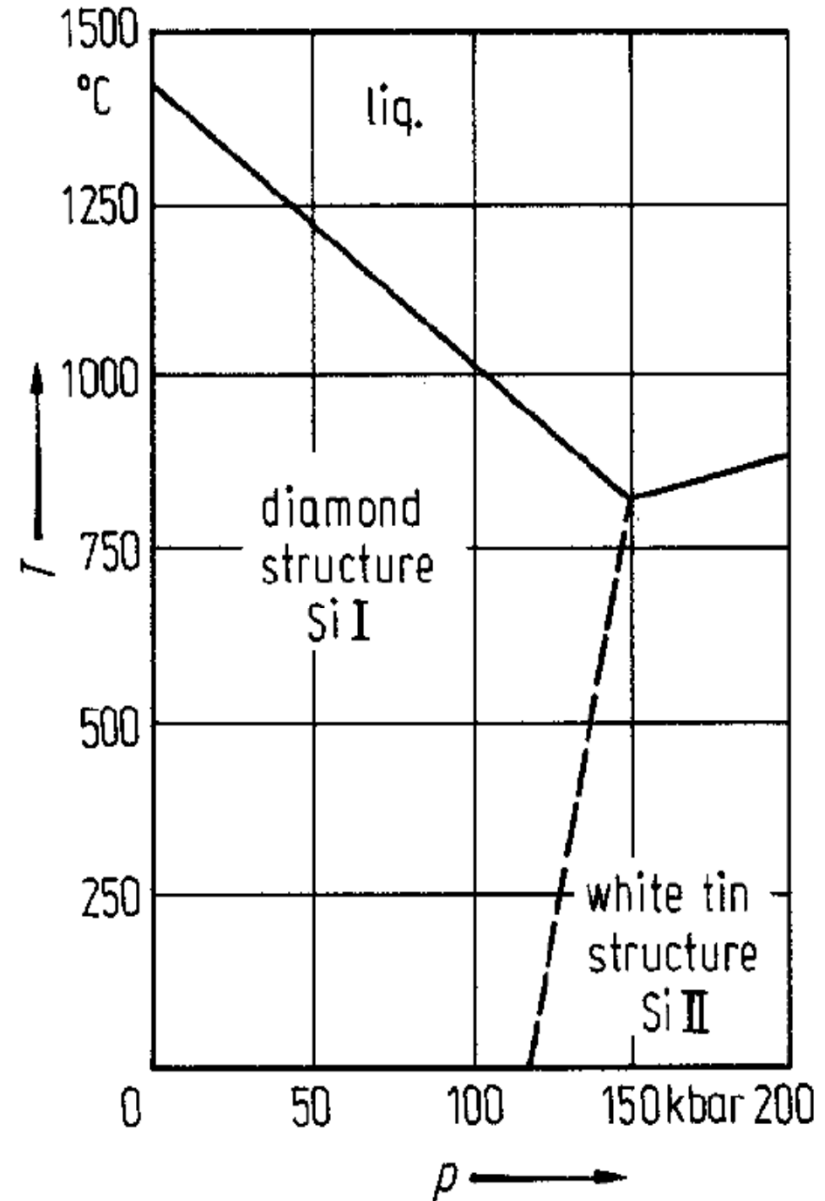


Si, diamond structure



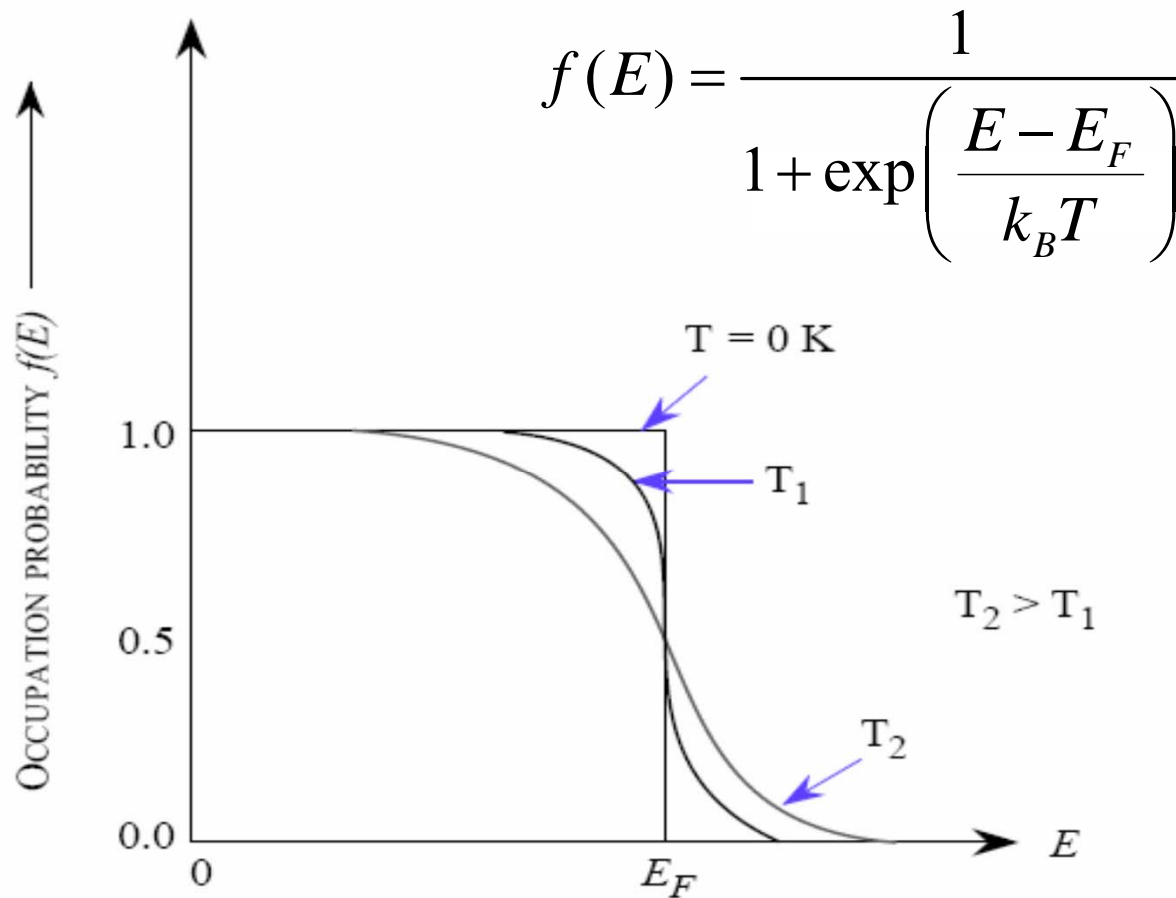
Si II,  $\beta$ -Sn, tetragonal

silicon makes a diamond to  $\beta$ -Sn transition under pressure



# Fermi function

$f(E)$  is the probability that a state at energy  $E$  is occupied.



# Silicon density of states

