

# 2. Intrinsic semiconductors

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Oct. 10, 2018

# Crystal Structure

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Atoms are arranged in a periodic pattern in a crystal.

The atomic arrangement affects the macroscopic properties of a material.

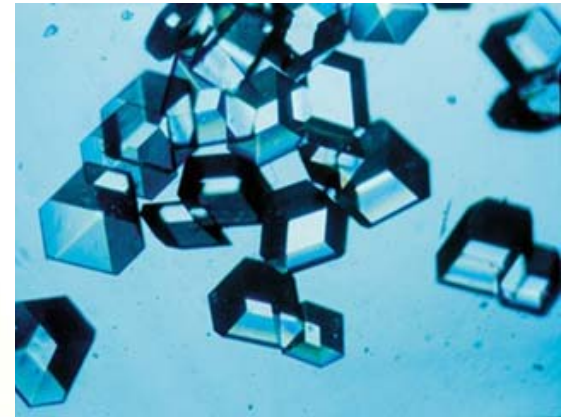
Many important materials (silicon, steel) are crystals



Gallium crystals



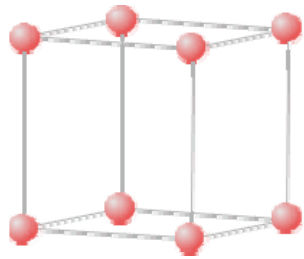
quartz



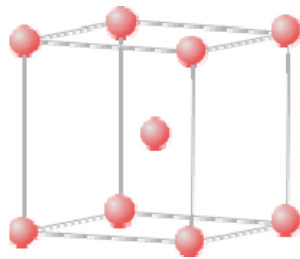
Insulin crystals

# Crystal Structure

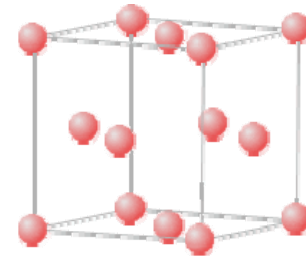
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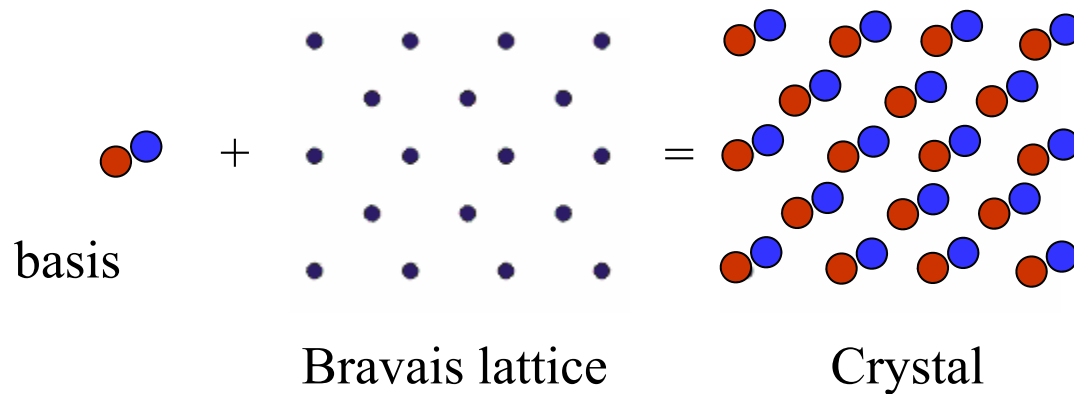
simple cubic



body centered  
cubic, bcc



face centered  
cubic, fcc

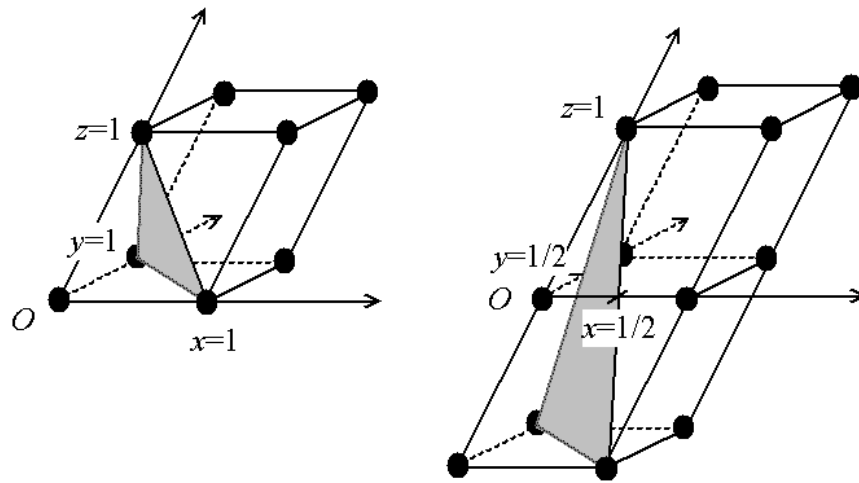
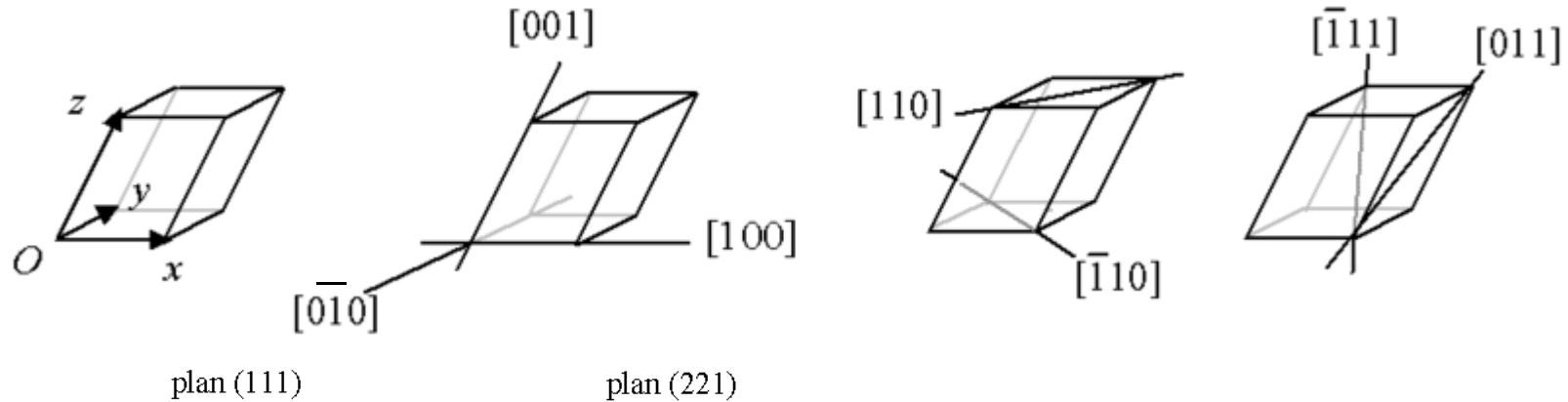


basis

Bravais lattice

Crystal

# Crystal planes and directions: Miller indices



A plane with the intercepts  $1/h$ ,  $1/k$ ,  $1/l$  is the  $(h,k,l)$  plane.

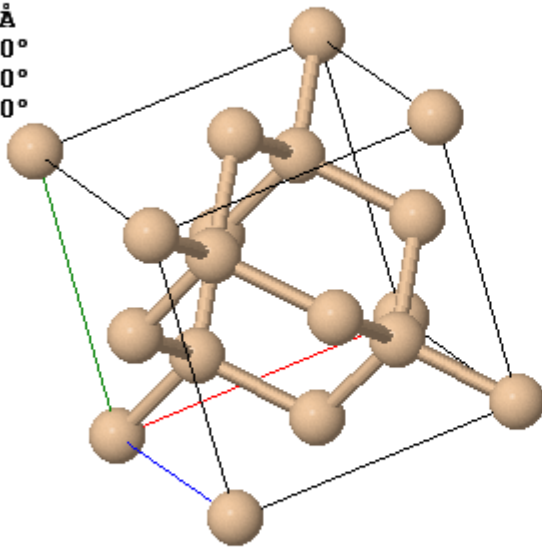
- [ ] specific direction
- < > family of equivalent directions
- () specific plane
- { } family of equivalent planes



MOSFETs are made on <100> wafers

# silicon

HM:  $F d \bar{3} m S$   
 $a=5.430\text{\AA}$   
 $b=5.430\text{\AA}$   
 $c=5.430\text{\AA}$   
 $\alpha=90.000^\circ$   
 $\beta=90.000^\circ$   
 $\gamma=90.000^\circ$



Conventional unit cell    Primitive unit cell    Asymmetric unit

2 x 2 x 2     3 x 3 x 3     5 x 5 x 5

Ball and Stick     Spacefill

H:     K:     L:

show HKL plane     hide HKL plane

draw atoms in HKL plane

Thickness of HKL planes:

The conventional unit cell is a cube with sides of 0.543 nm. There are 8 atoms in the conventional unit cell. (The image can be rotated with a mouse.)

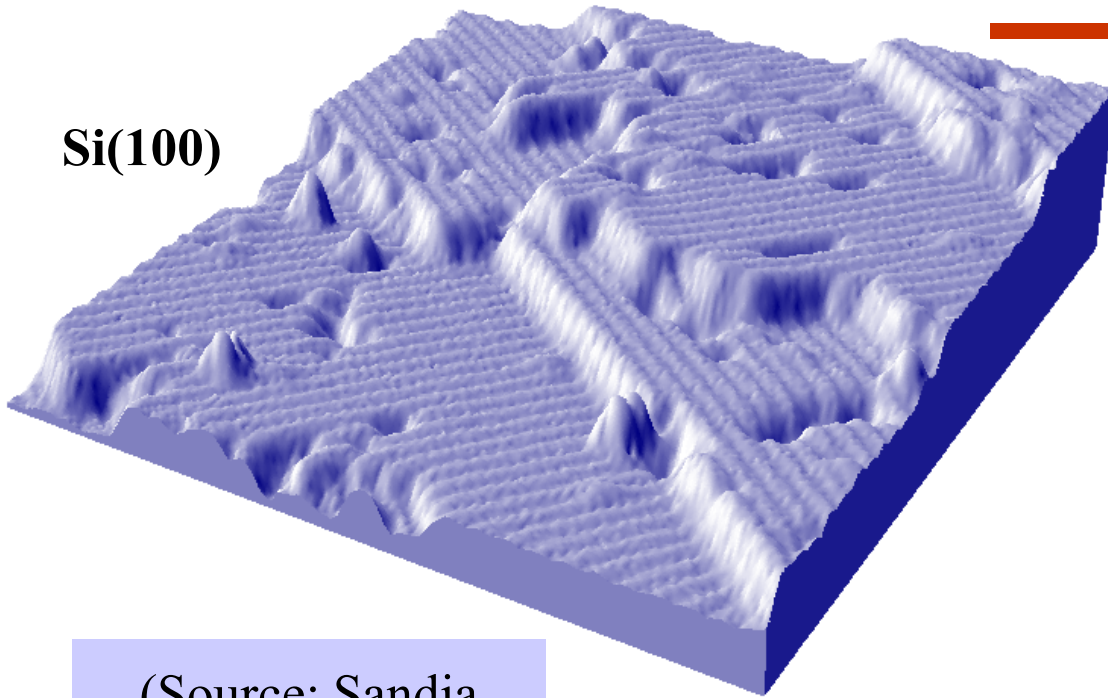
JSmol

<http://lampx.tugraz.at/~hadley/memmm/materials/silicon/silicon.php>

# Silicon surfaces

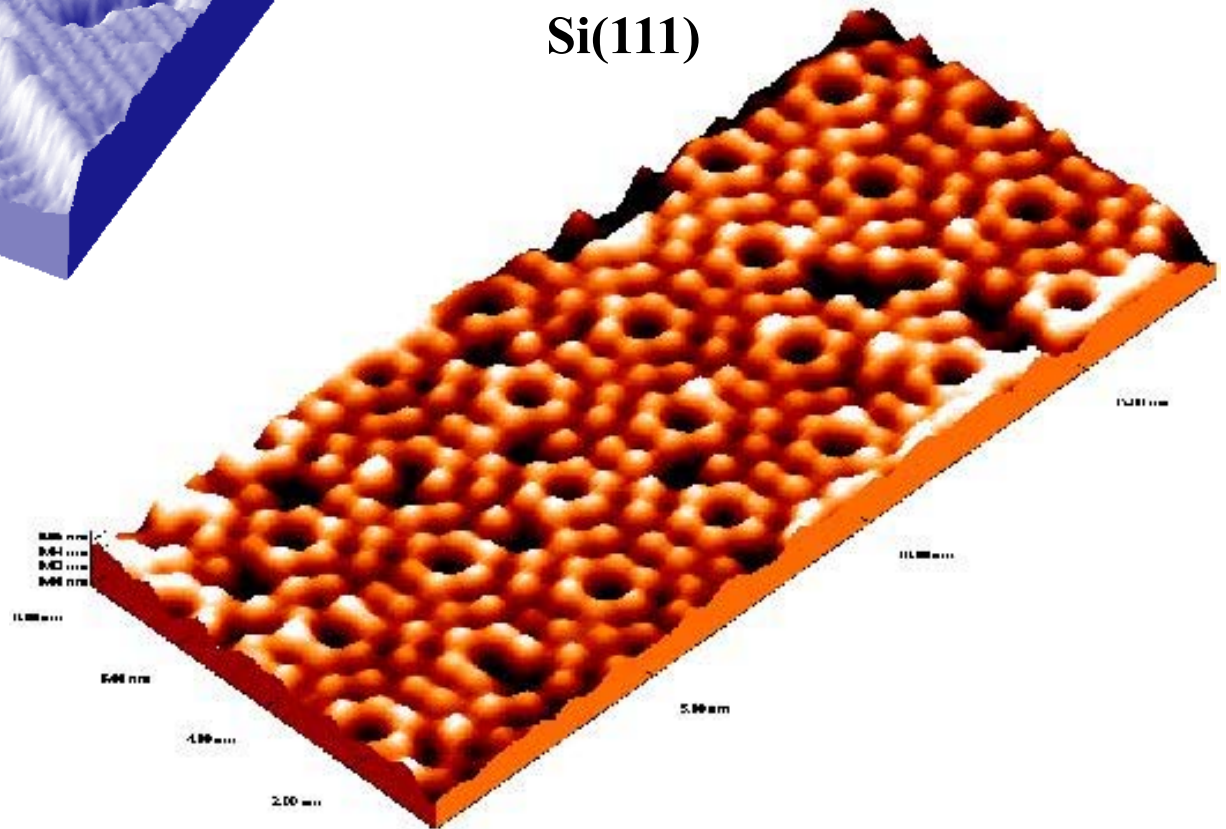
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Si(100)



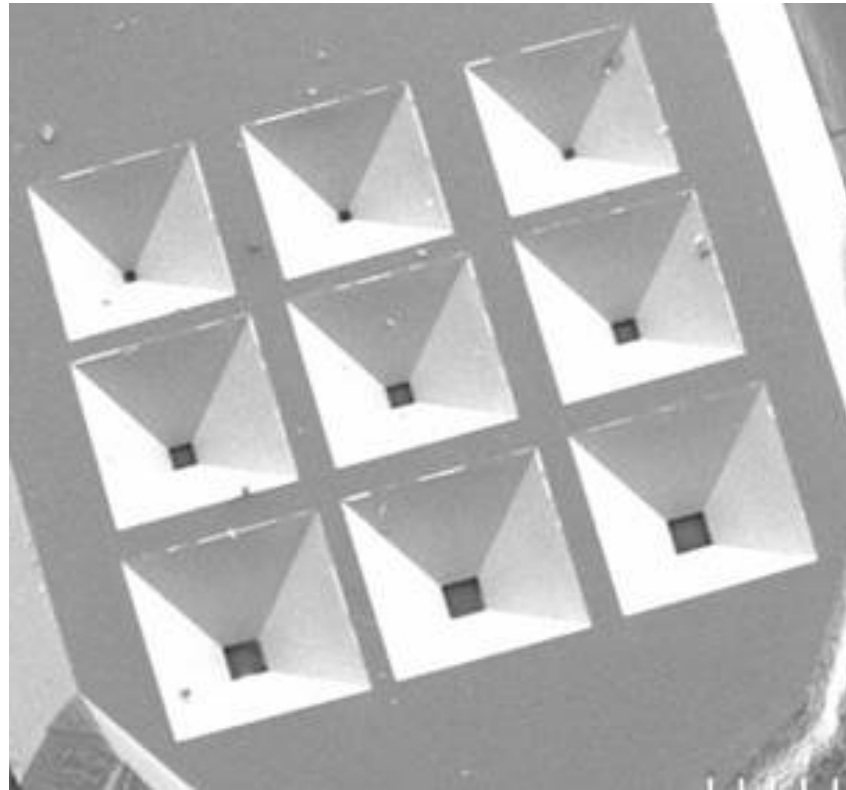
(Source: Sandia  
Nat.Labs.)

Si(111)



# KOH etching of silicon

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KOH etches Si  $\{110\} > \{100\} > \{111\}$ , producing a characteristic anisotropic V-etch, with sidewalls that form a  $54.7^\circ$  angle with the surface ( $35.3^\circ$  from the normal).

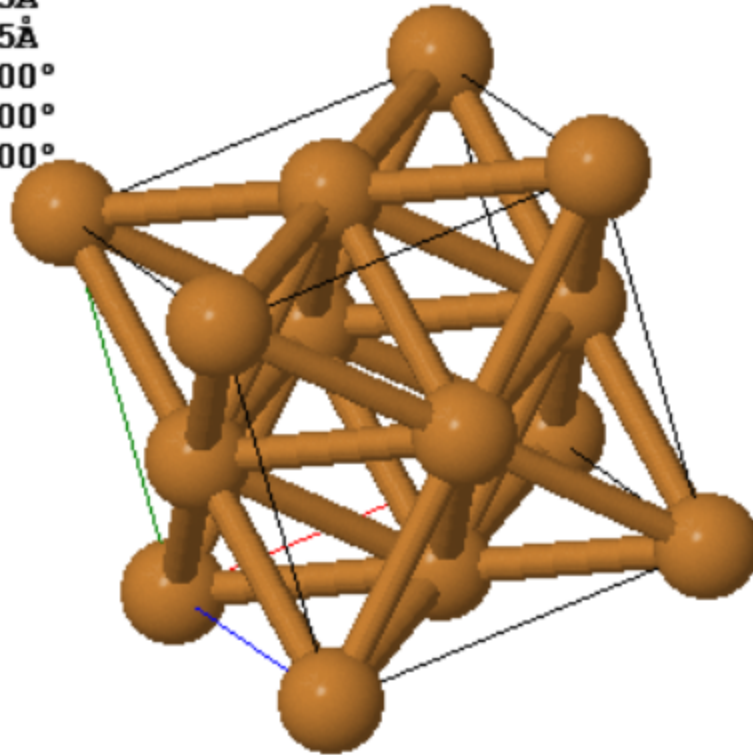
[http://www.ece.uncc.edu/research/clean\\_room/fabprocesses/KOH-EtchingAndDecon.pdf](http://www.ece.uncc.edu/research/clean_room/fabprocesses/KOH-EtchingAndDecon.pdf)



# face centered cubic (fcc)

Al, Cu,  
Ni, Ag,  
Pt, Au,  
Pb

HM:  $F m \bar{3} m$   
 $a=3.615\text{\AA}$   
 $b=3.615\text{\AA}$   
 $c=3.615\text{\AA}$   
 $\alpha=90.000^\circ$   
 $\beta=90.000^\circ$   
 $\gamma=90.000^\circ$



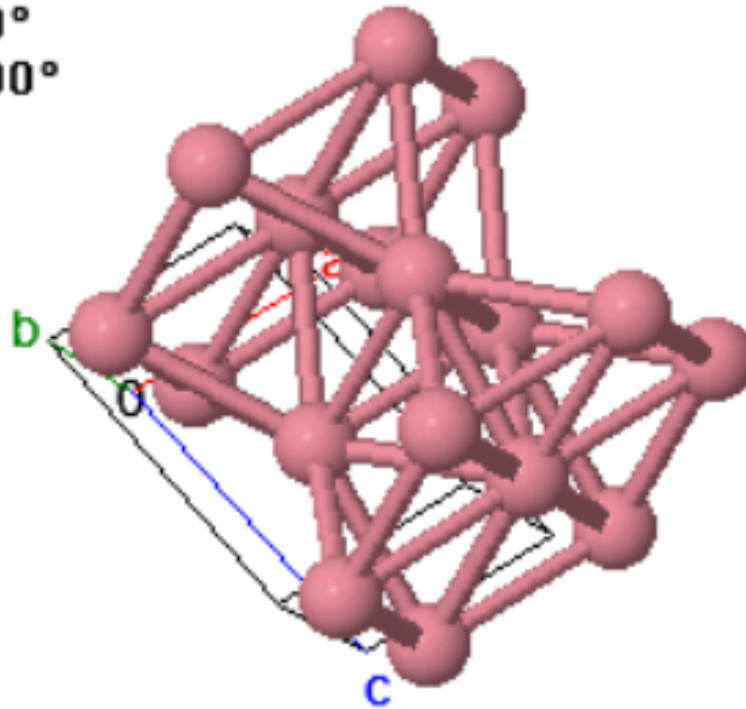
[http://lampx.tugraz.at/~hadley/ss1/crystalstructure/structures/fcc/fcc\\_jsmol.php](http://lampx.tugraz.at/~hadley/ss1/crystalstructure/structures/fcc/fcc_jsmol.php)



# hexagonal close pack (hcp)

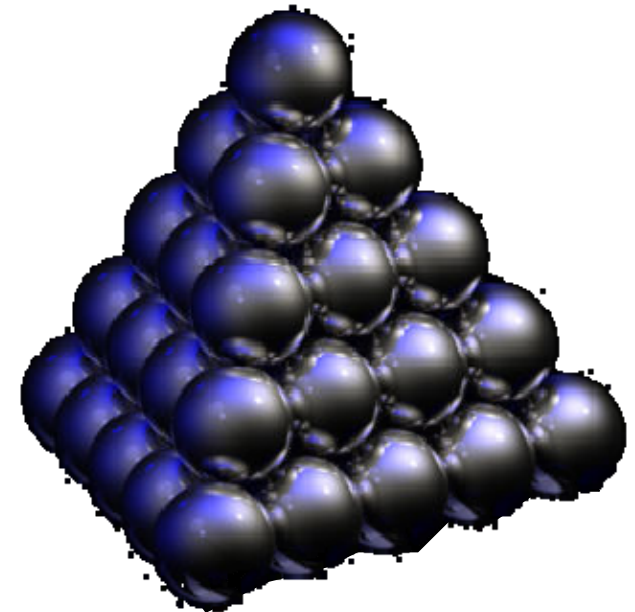
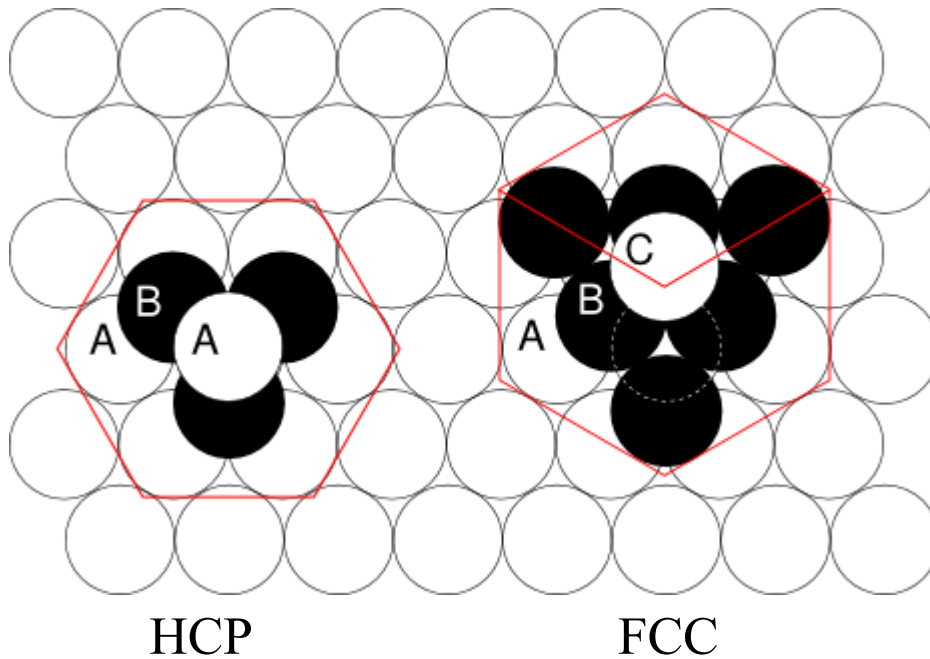
Ti, Co,  
Zn, Zr,

HM: P 63/m m c  
a=2.507Å  
b=2.507Å  
c=4.069Å  
 $\alpha=90.000^\circ$   
 $\beta=90.000^\circ$   
 $\gamma=120.000^\circ$



# Close packing

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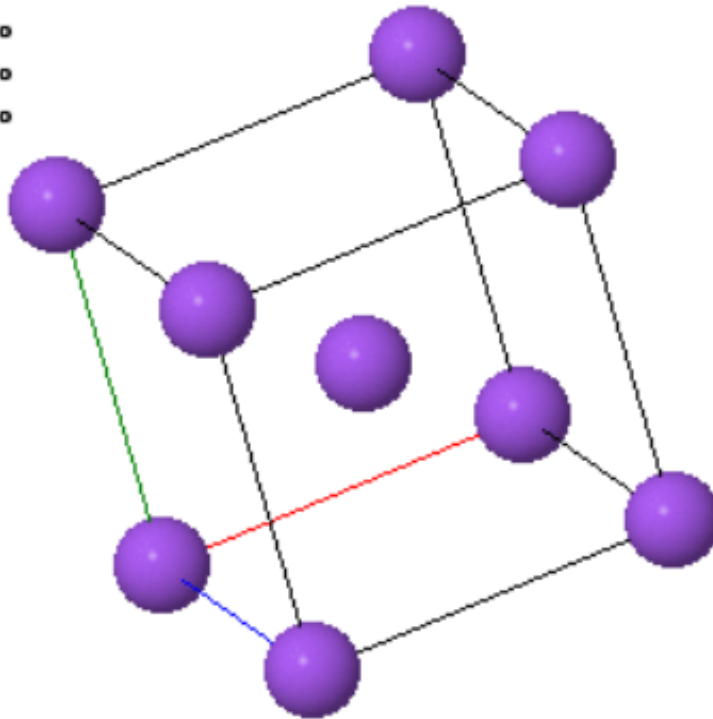
HCP = Hexagonal close pack

Hexagonal Bravais lattice with two atoms in the basis.

# body centered cubic bcc

W  
Cr  
Fe  
Mo  
Ta

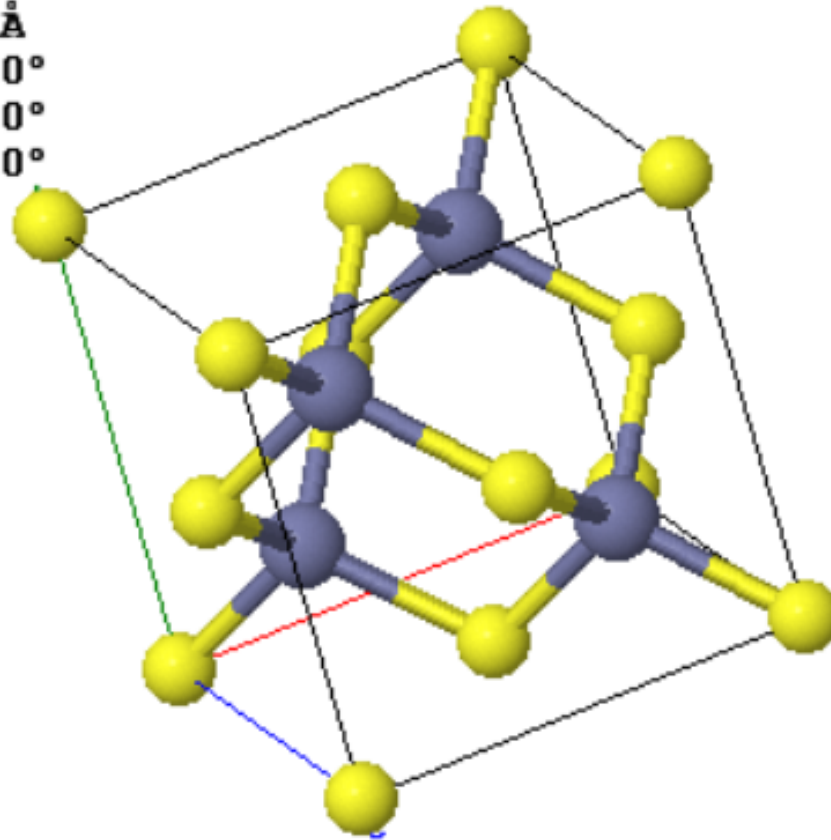
HM: IM-3M  
a=4.291Å  
b=4.291Å  
c=4.291Å  
α=90.000°  
β=90.000°  
γ=90.000°



# zincblende

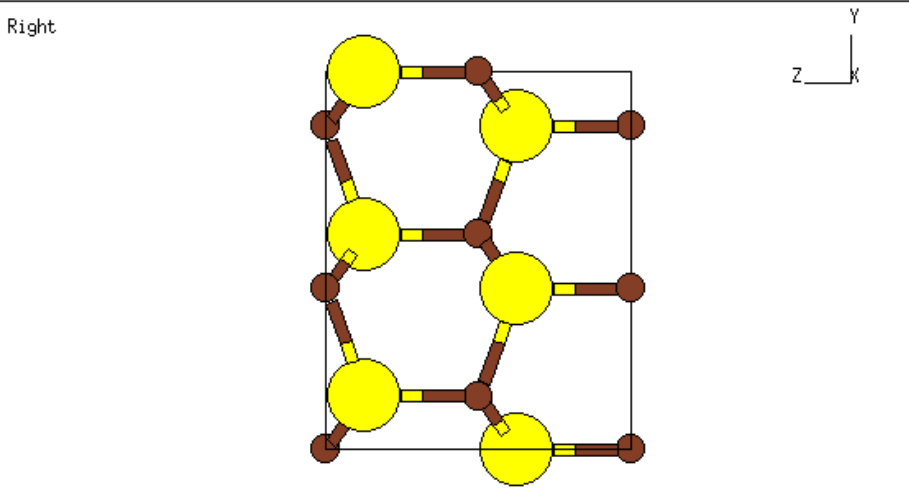
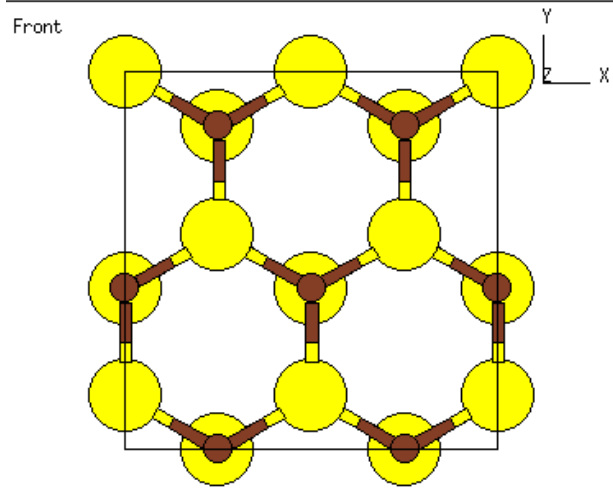
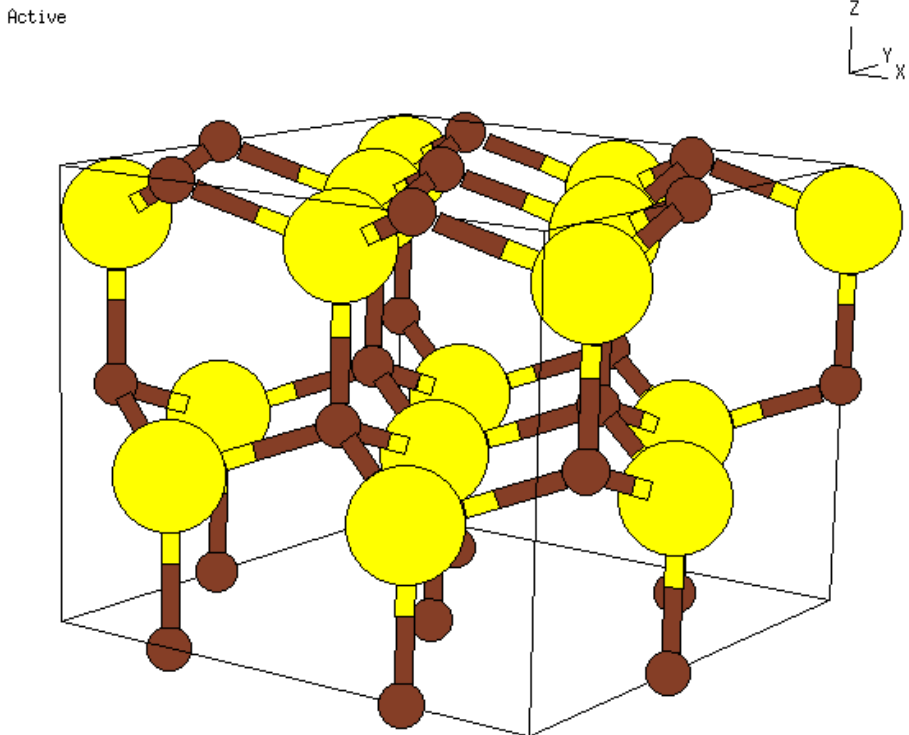
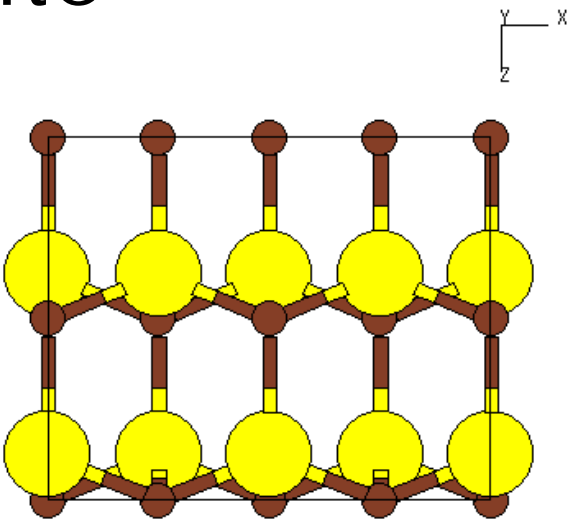
ZnS  
GaAs  
InP  
GaP  
InAs  
AlAs

HM: F-43M  
a=5.434Å  
b=5.434Å  
c=5.434Å  
α=90.000°  
β=90.000°  
γ=90.000°



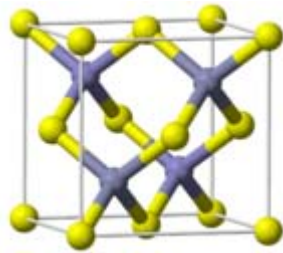
# wurtzite

- ZnO
- CdS
- CdSe
- GaN
- AlN



# Structural phase transitions

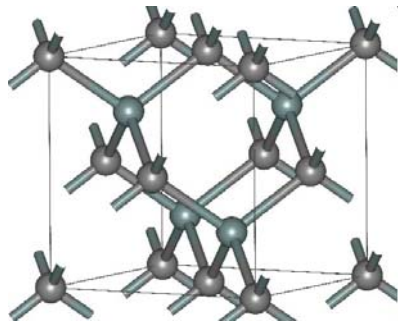
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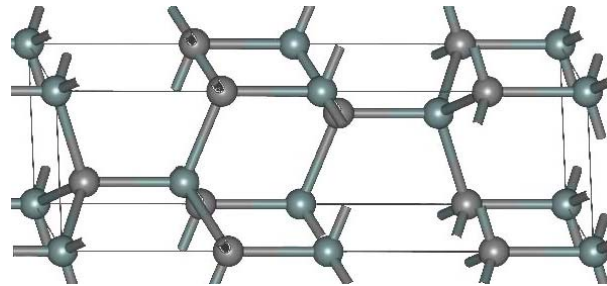
GaAs, Zinblende



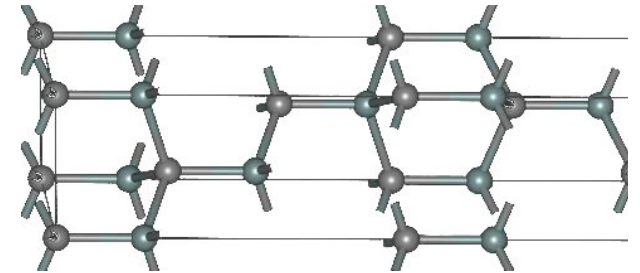
GaAs, Wurtzite



3C - SiC



4H - SiC



6H - SiC

SiC has about 100 polytypes

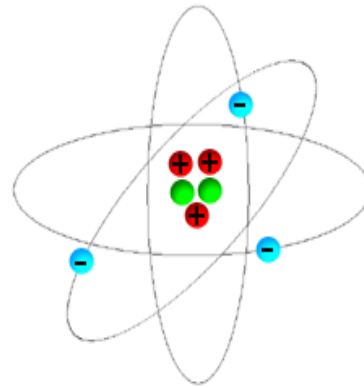
# Electrons

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

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

Radius = ?



0.15 nm

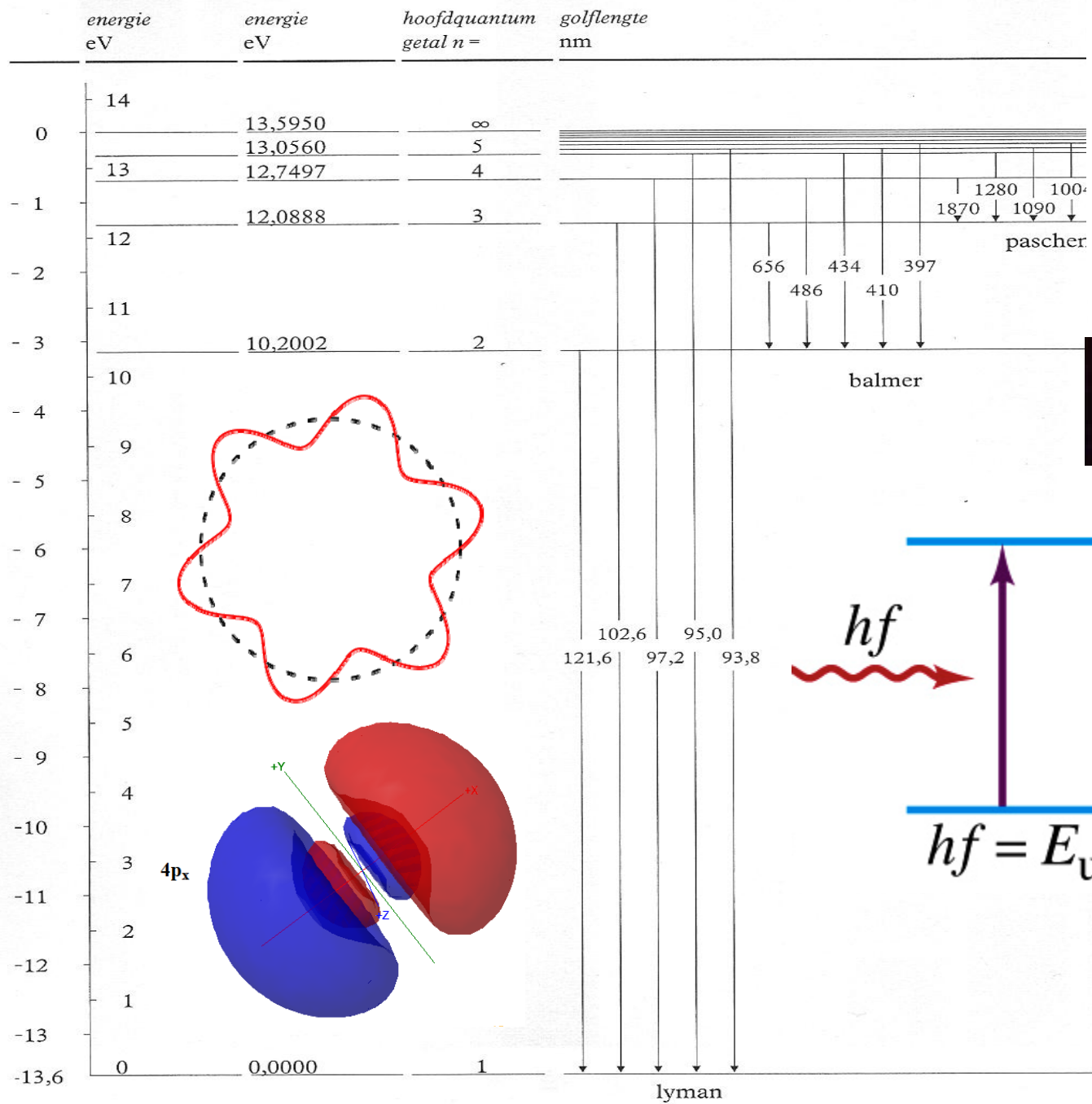


[www.alnaden.ibm.com/vis/stm/atomo.html](http://www.alnaden.ibm.com/vis/stm/atomo.html)

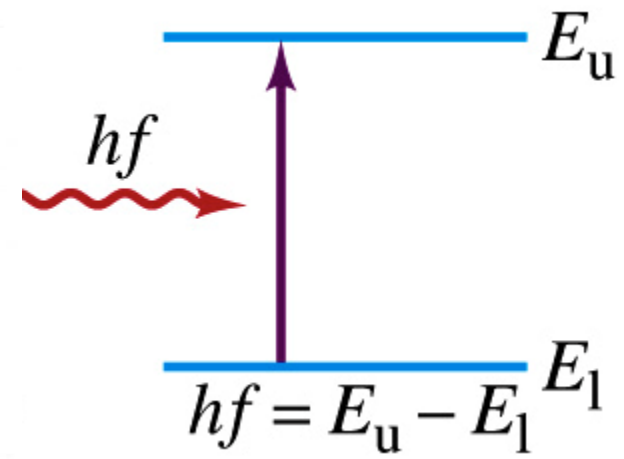
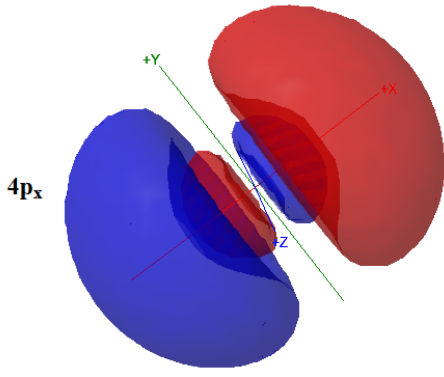
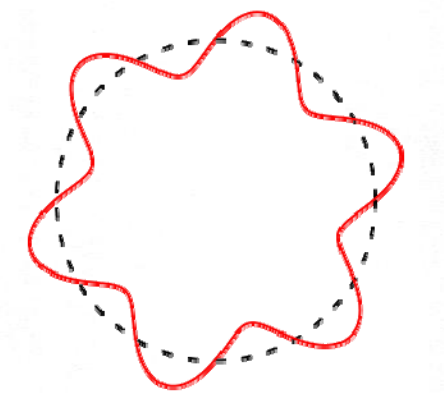
# Quantum Mechanics

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

de aangegeven golflengten gelden in vacuüm

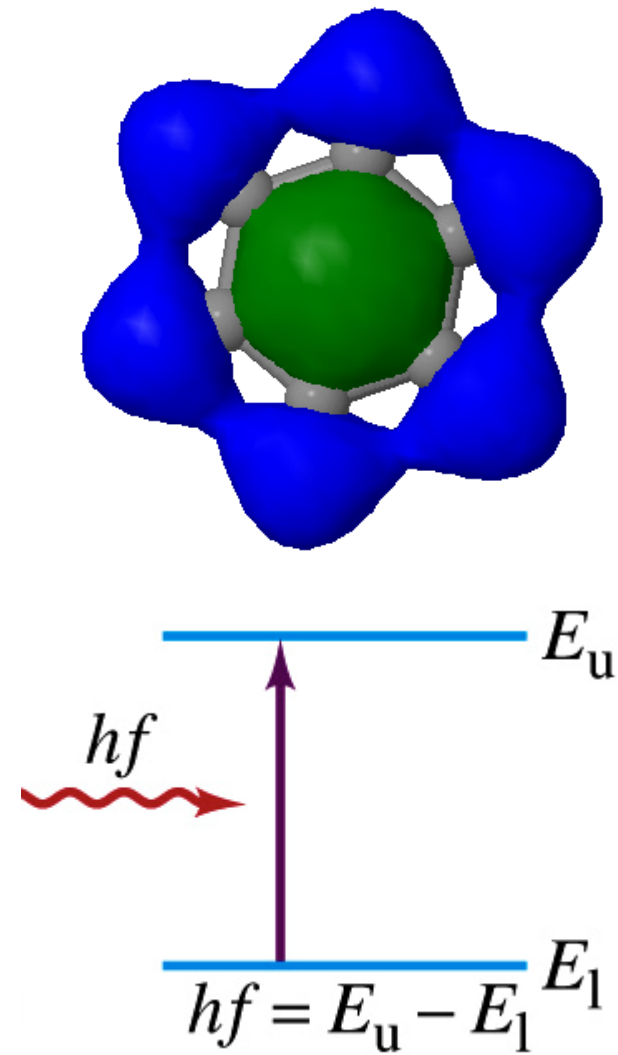
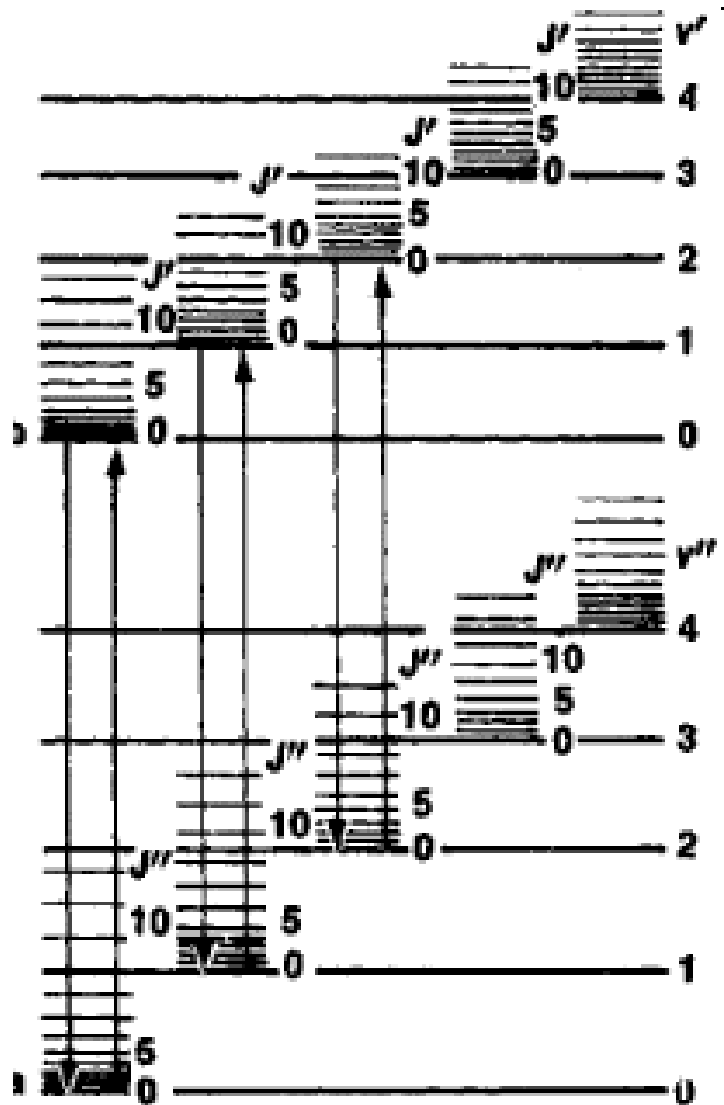


Fluorescent lamp



lyman

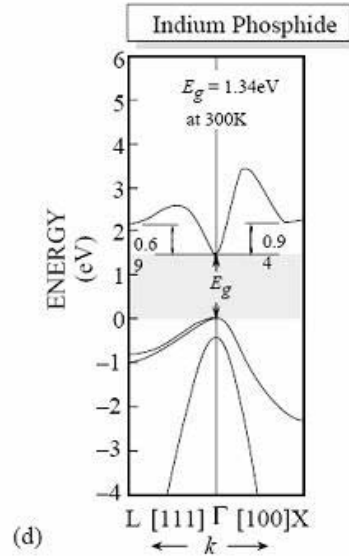
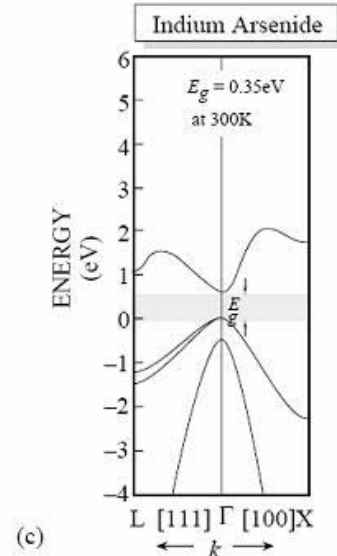
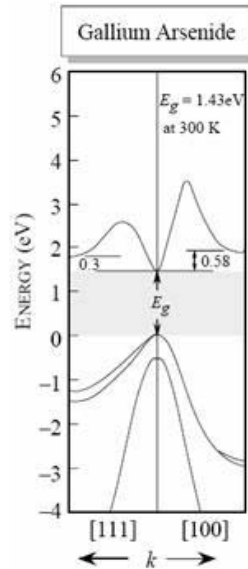
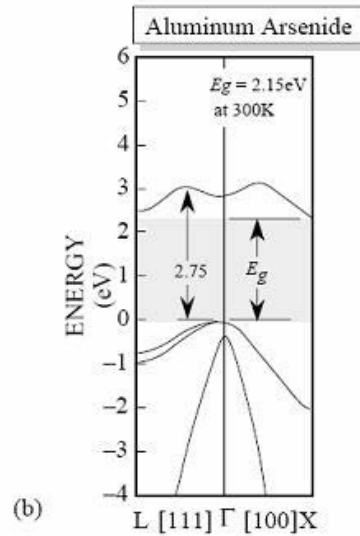
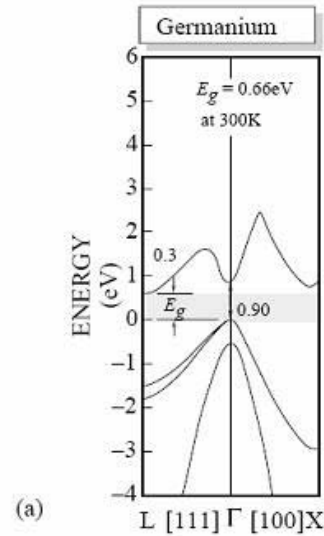
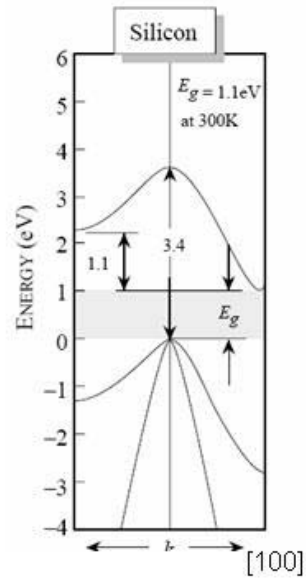
# Molecular energy levels



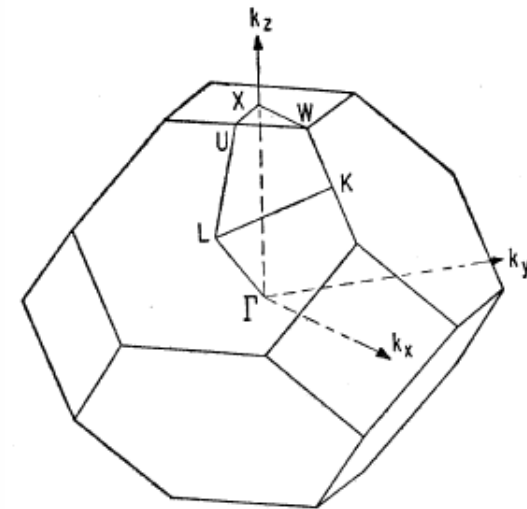
Everything moves like a wave but exchanges energy and momentum like a particle.



# Semiconductors



valence band  
 conduction band  
 band gap



molecular orbitals  
 are plane waves

# wave vector $k$

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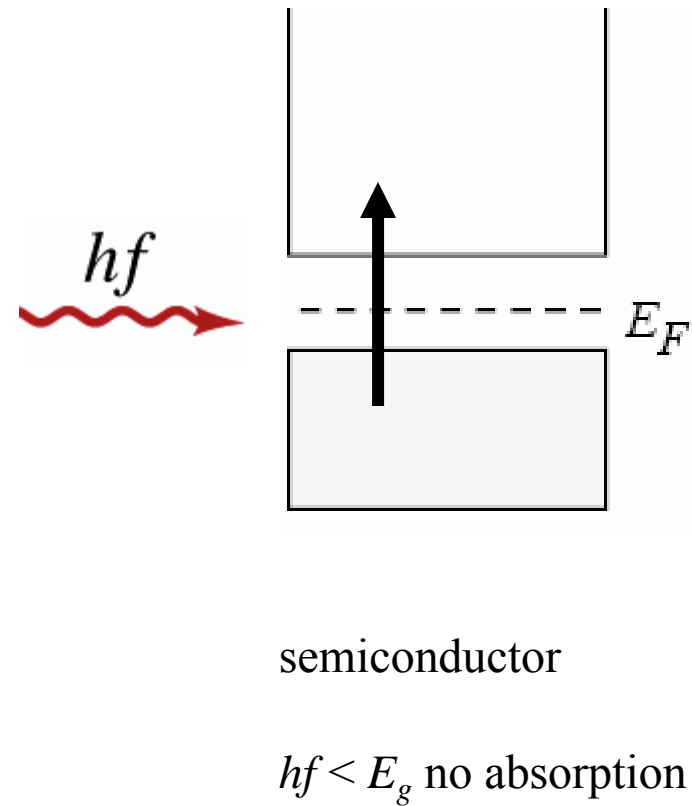
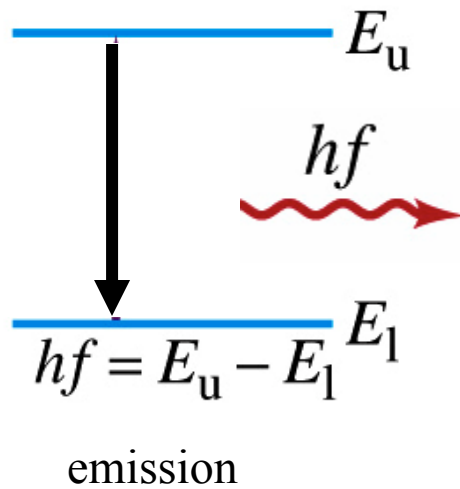
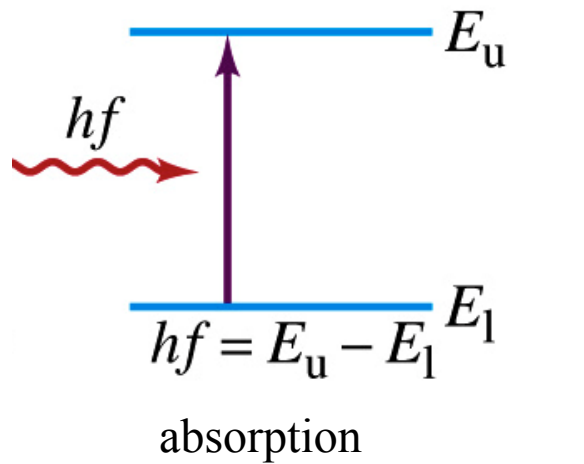
A  $k$ -vector points in the direction a wave is propagating.

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

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

# Absorption and emission of photons

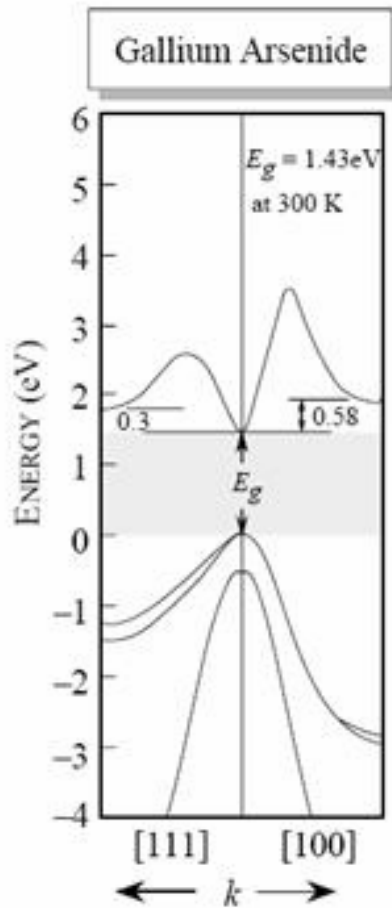
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# What color light does a GaAs LED emit?

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

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

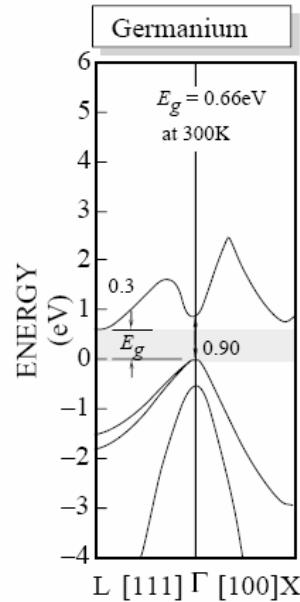
# Direct and indirect band gaps

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indirect bandgap

$$\Delta k \neq 0$$

phonons are emitted

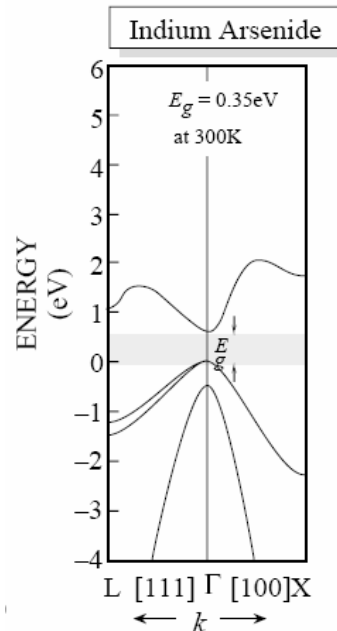


Momentum must be conserved when photons are absorbed or emitted.

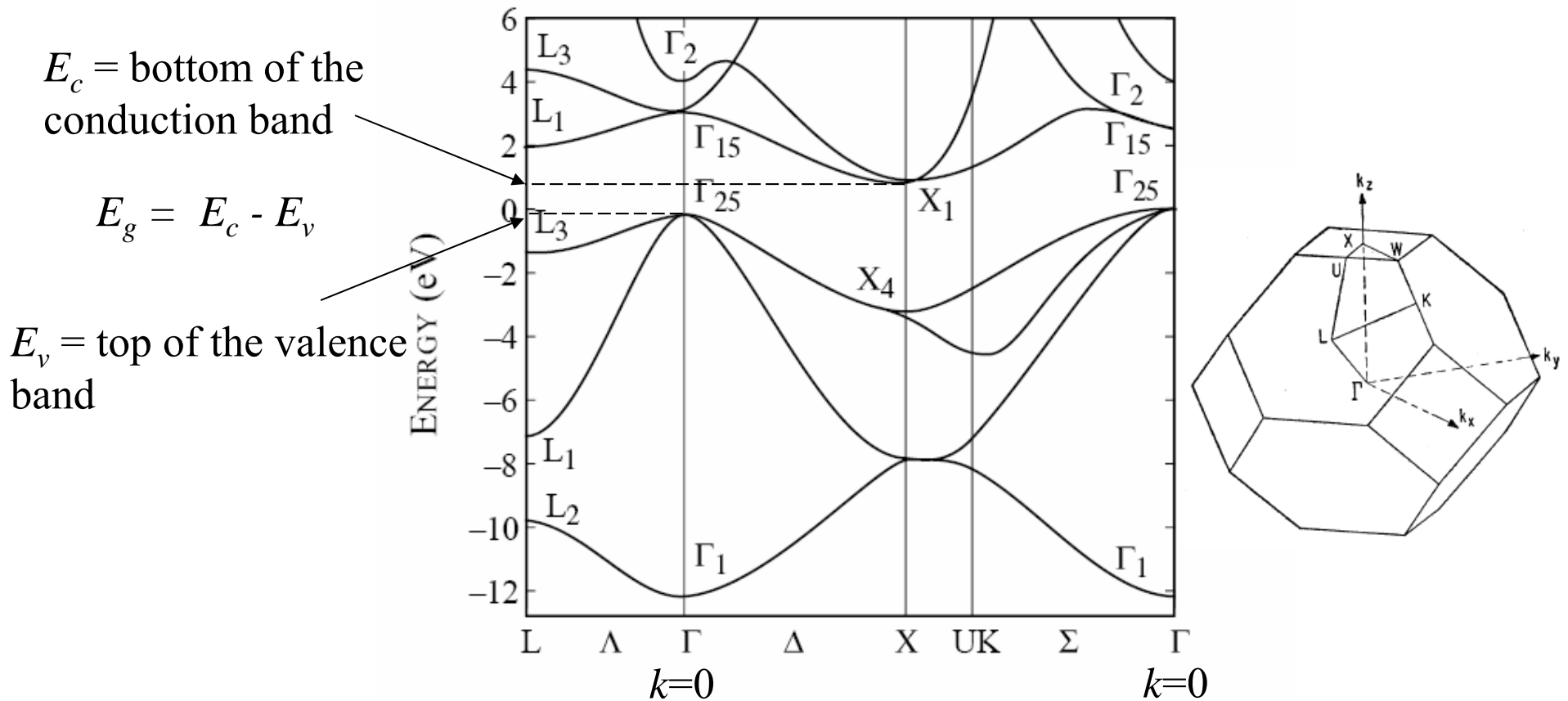
direct bandgap:

$$\Delta k = 0$$

photons can be emitted



# Silicon band structure

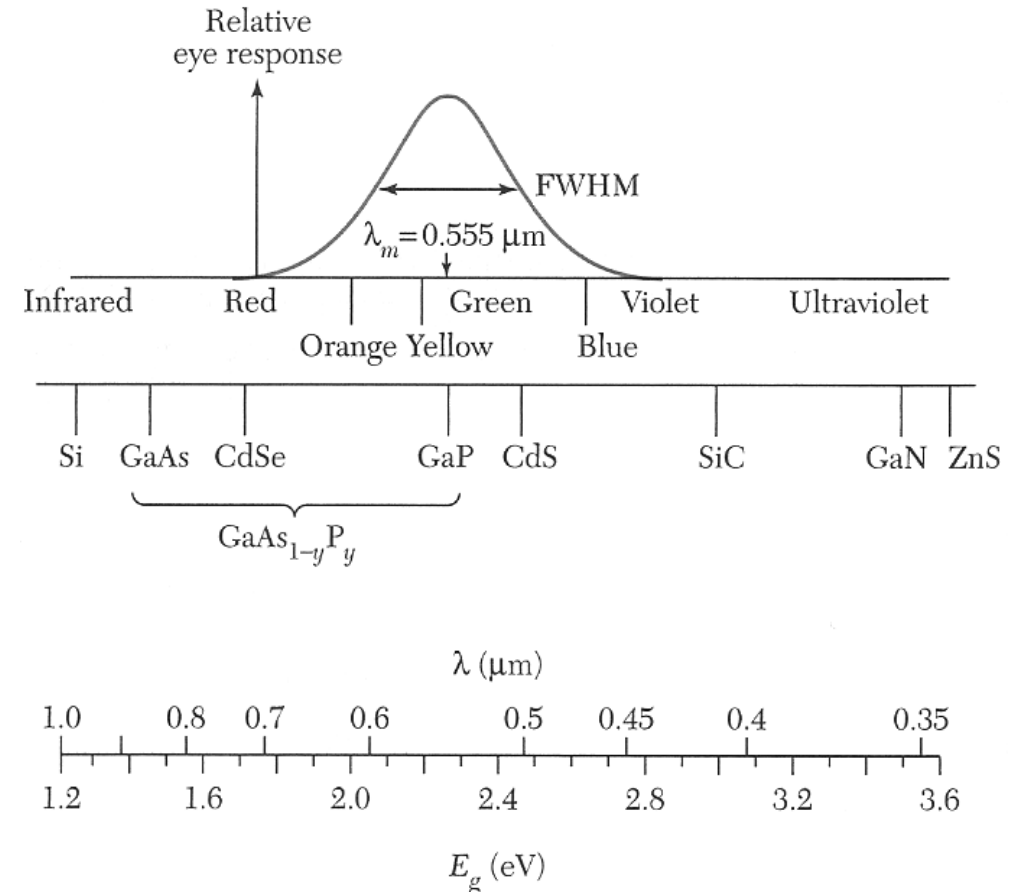


Electrons with energies in the gap are reflected out of the crystal.

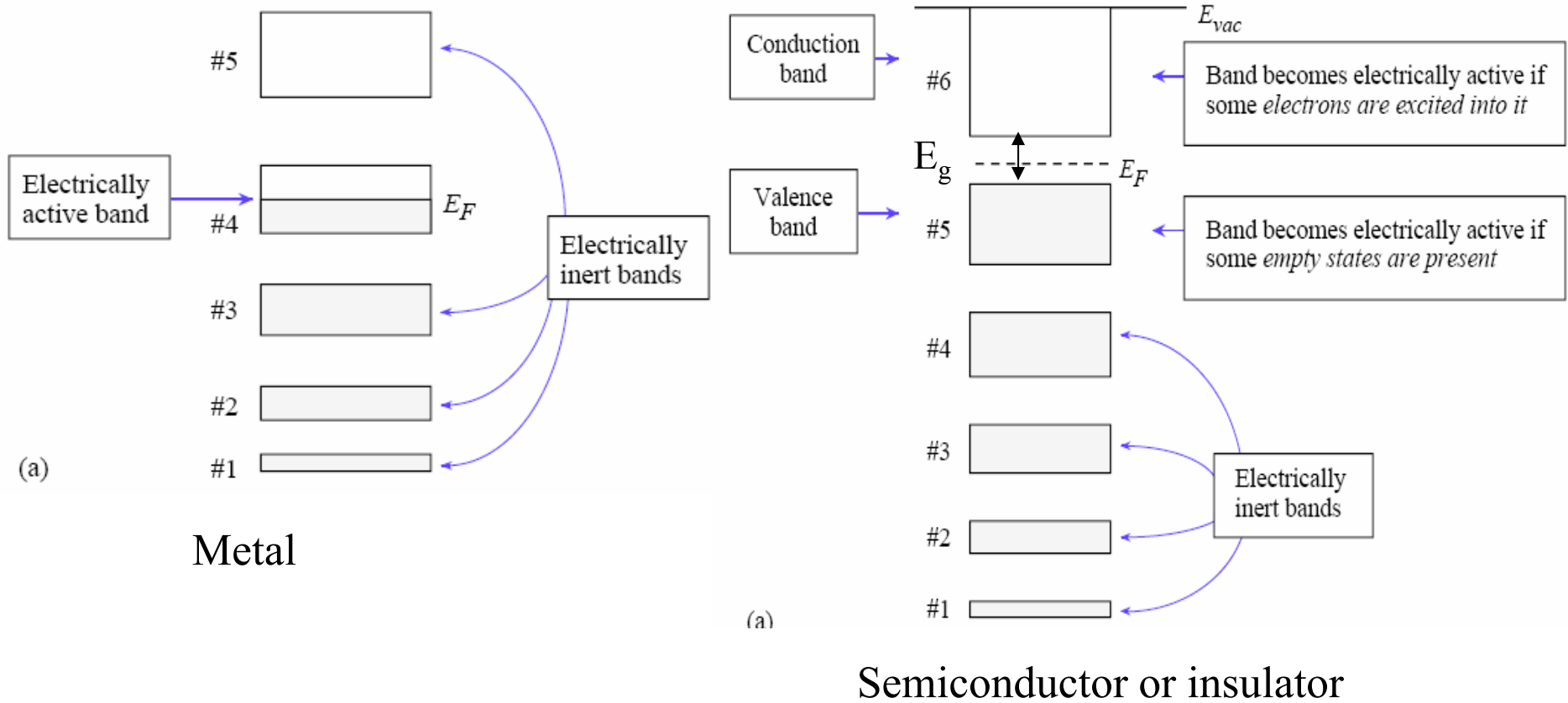
**TABLE 1 Common III-V materials used to produce LEDs and their emission wavelengths.**

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

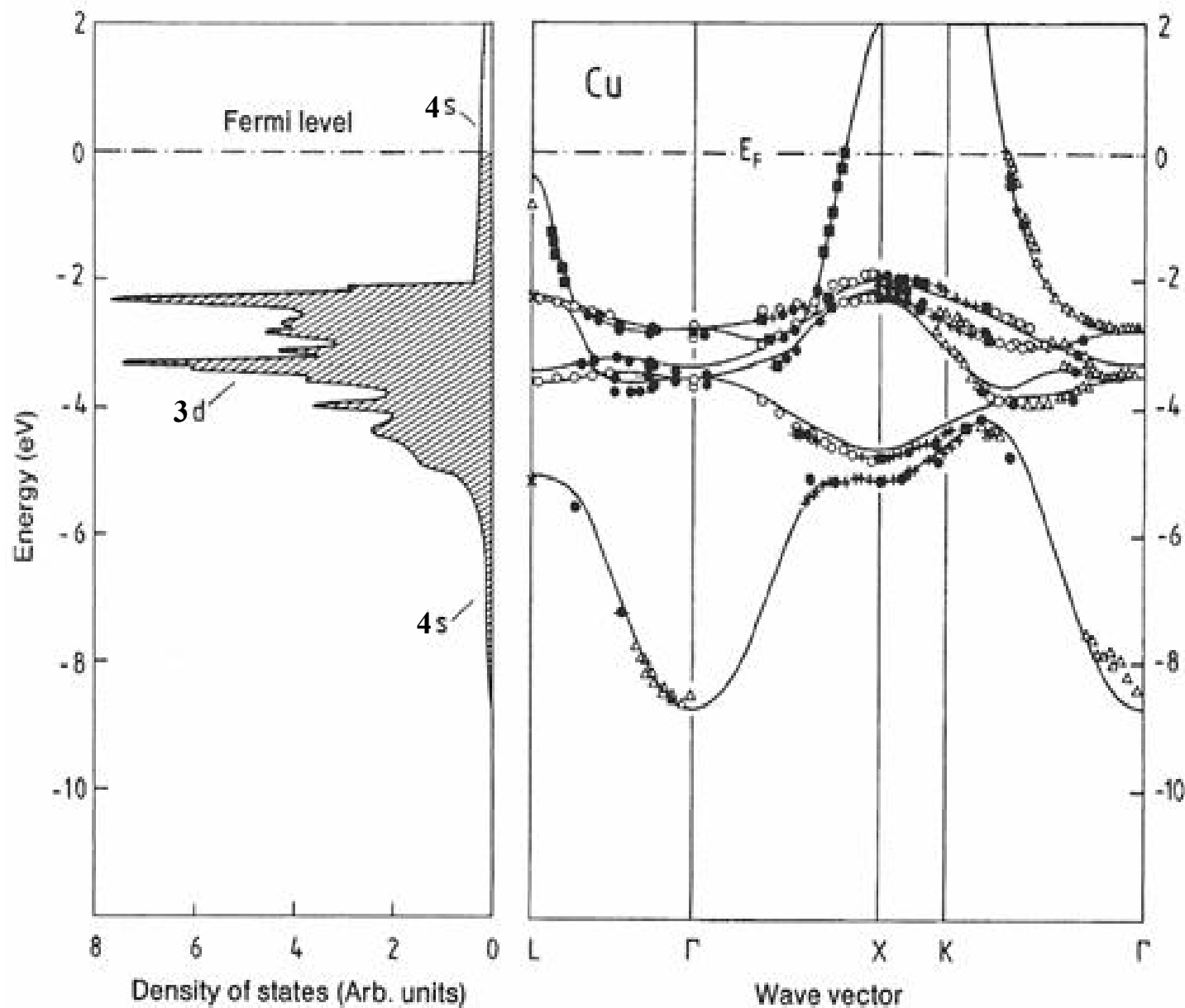


$E_g < 3\text{eV} = \text{Semiconductor}$

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

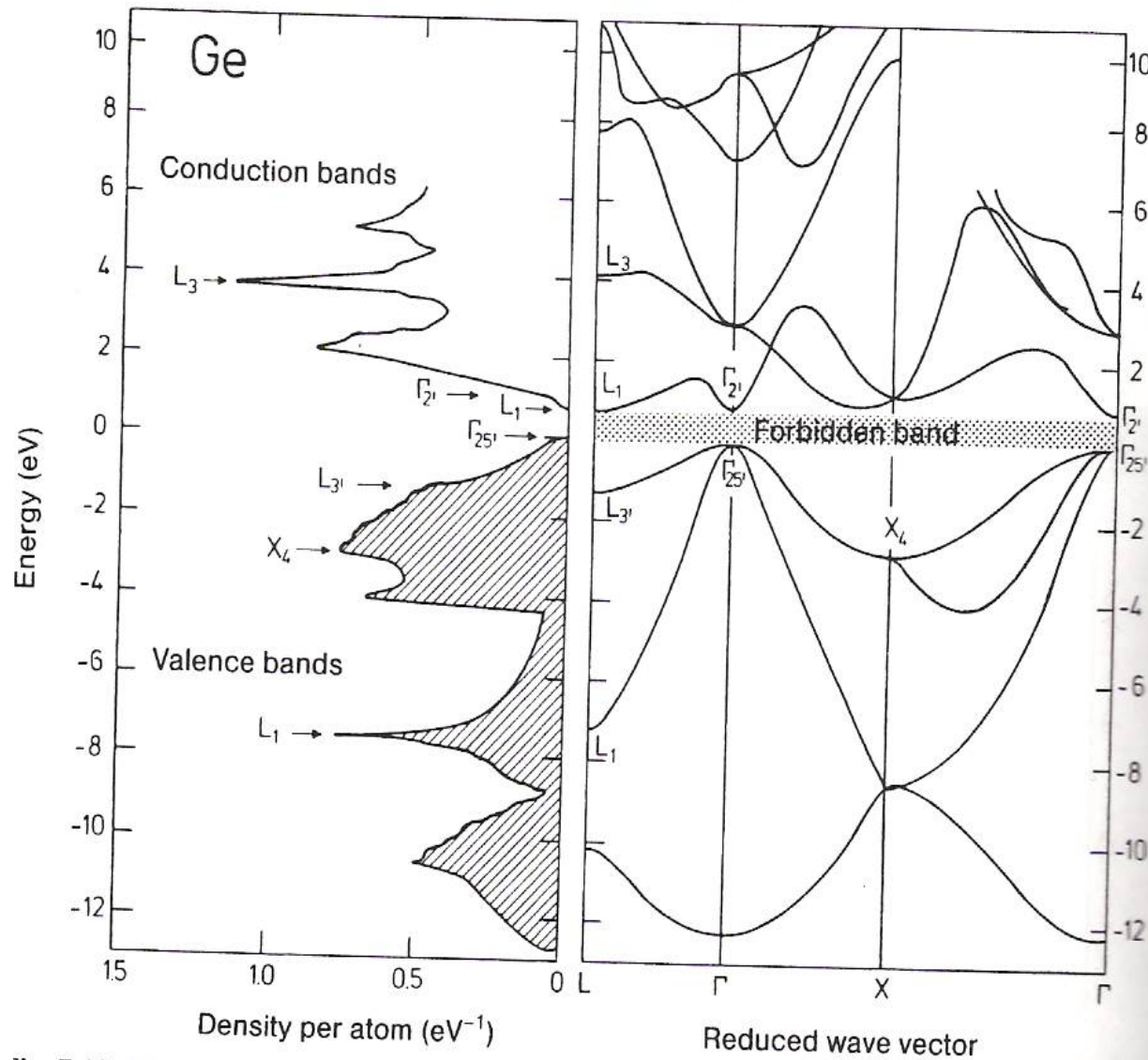
from: Singh

# Copper dispersion relation and density of states



from Ibach & Lueth

# Germanium

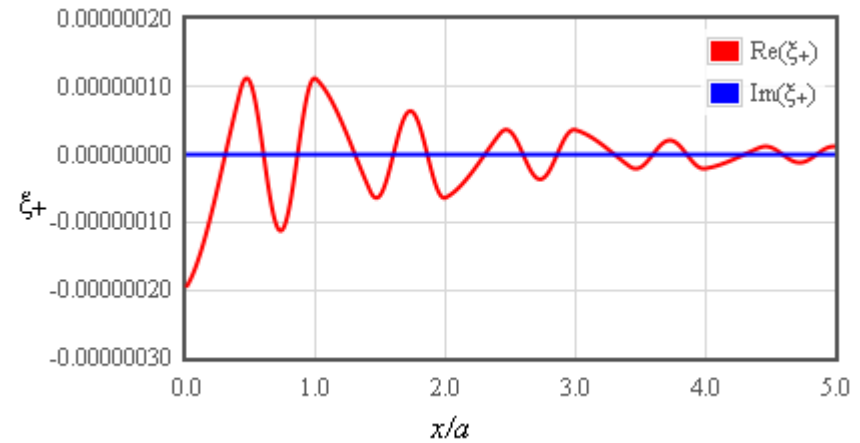
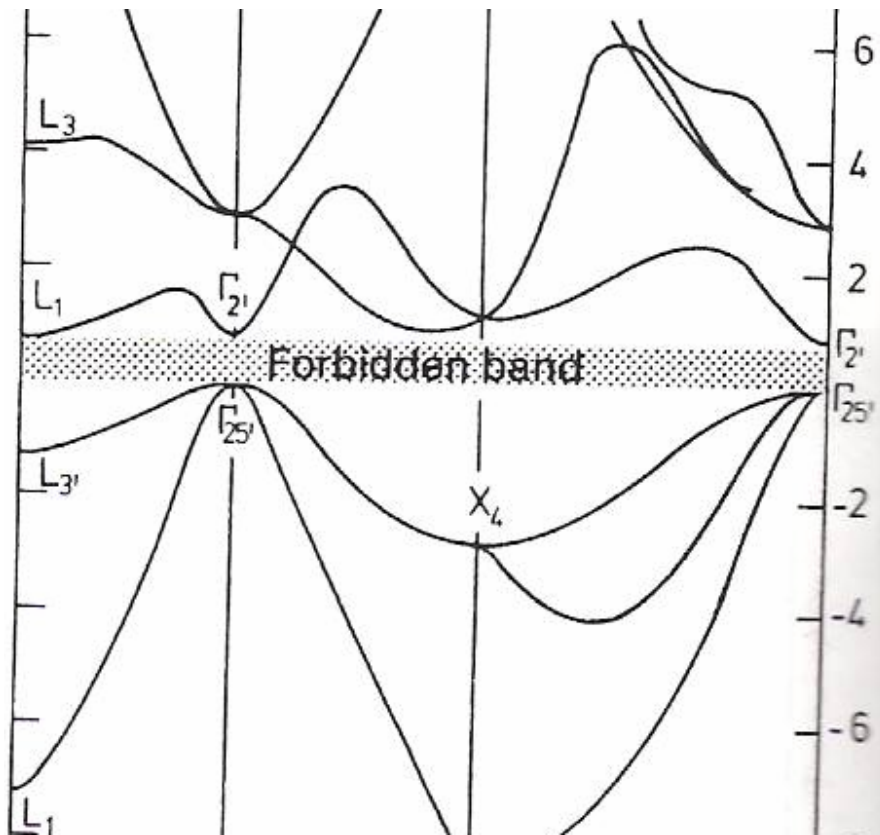


from Ibach & Lueth



# Band gap

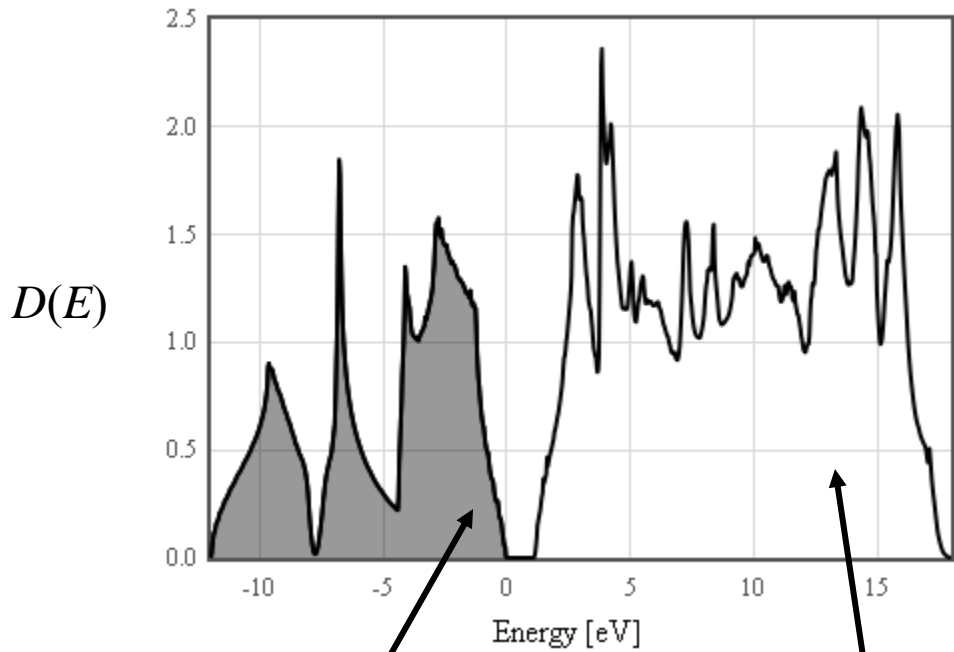
Electrons with energies in the gap are reflected out of the crystal.



# Density of states

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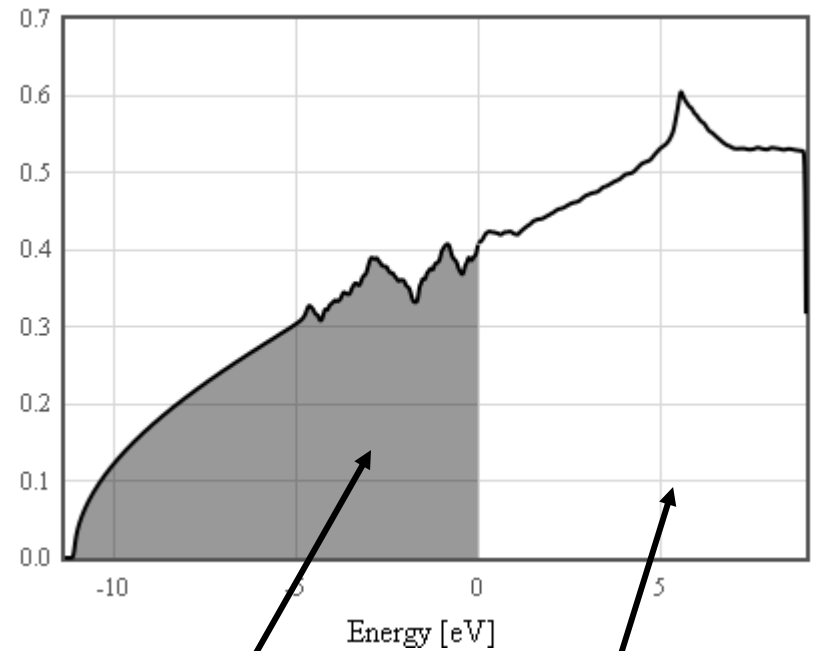
Silicon



filled states

empty states

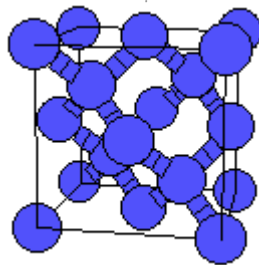
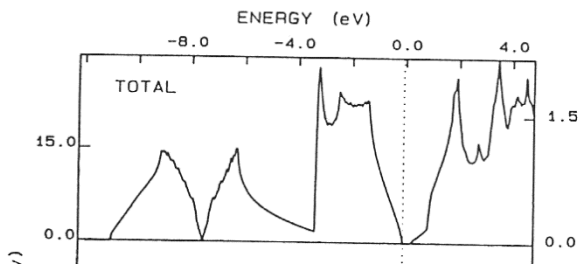
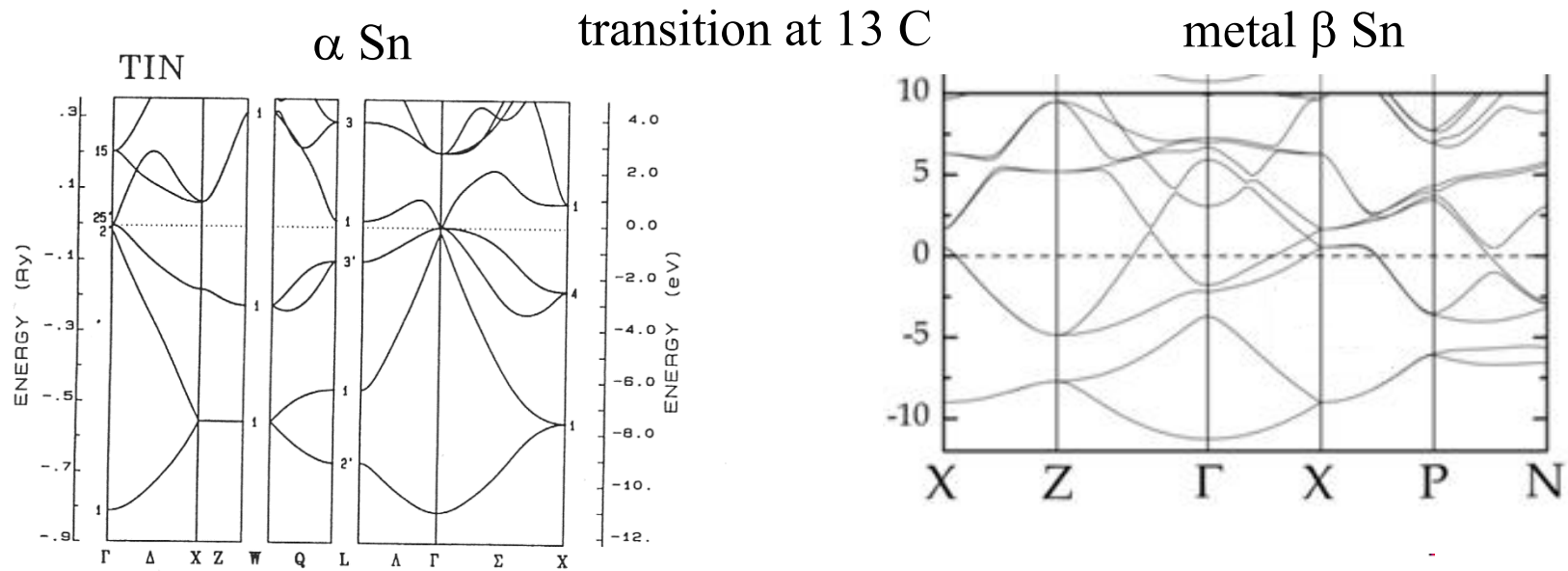
Aluminum



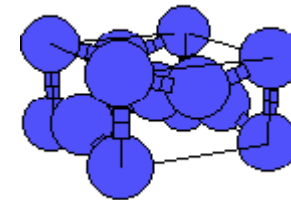
filled states

empty states

# Structural phase transition in Sn

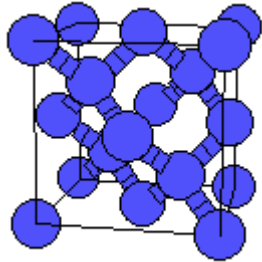


$\alpha$ -Sn, gray tin, diamond structure

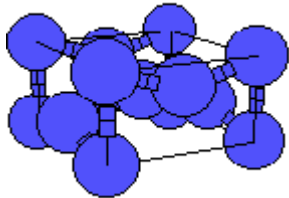


$\beta$ -Sn, white tin, tetragonal

# Structural phase transitions

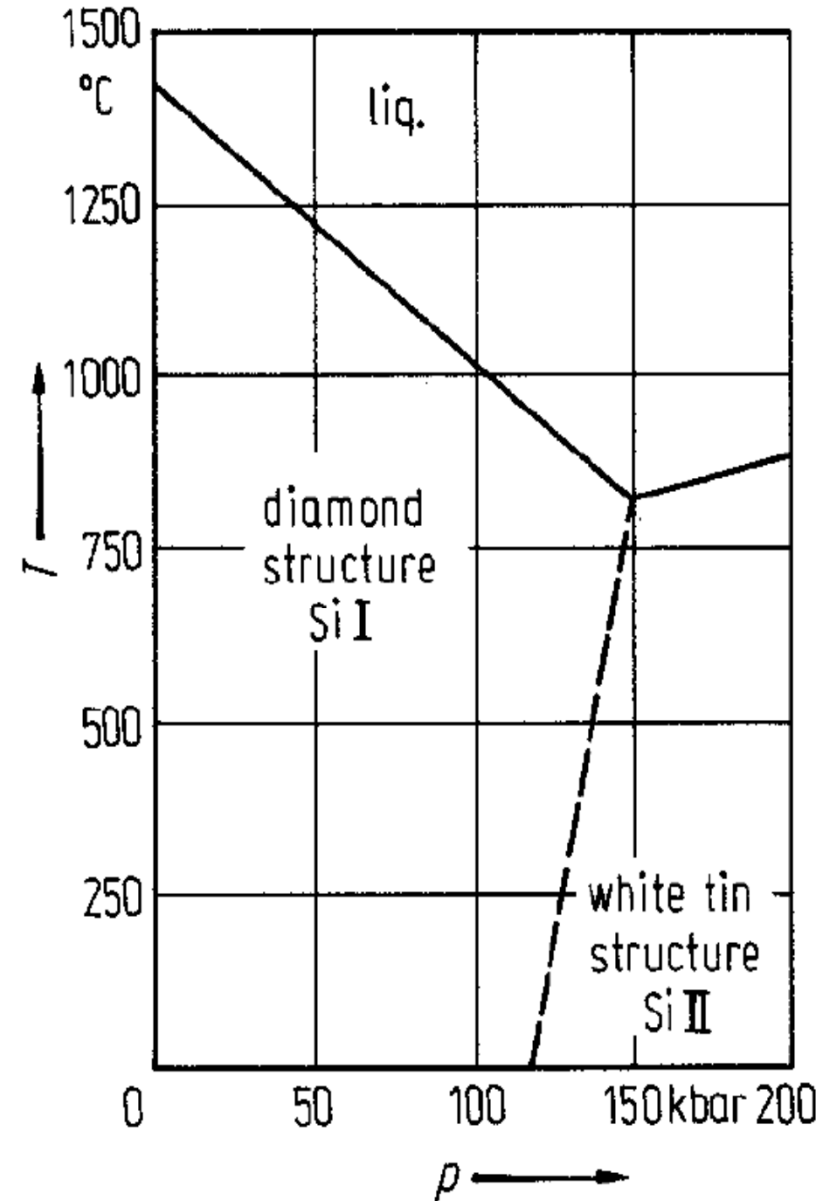


Si, diamond structure



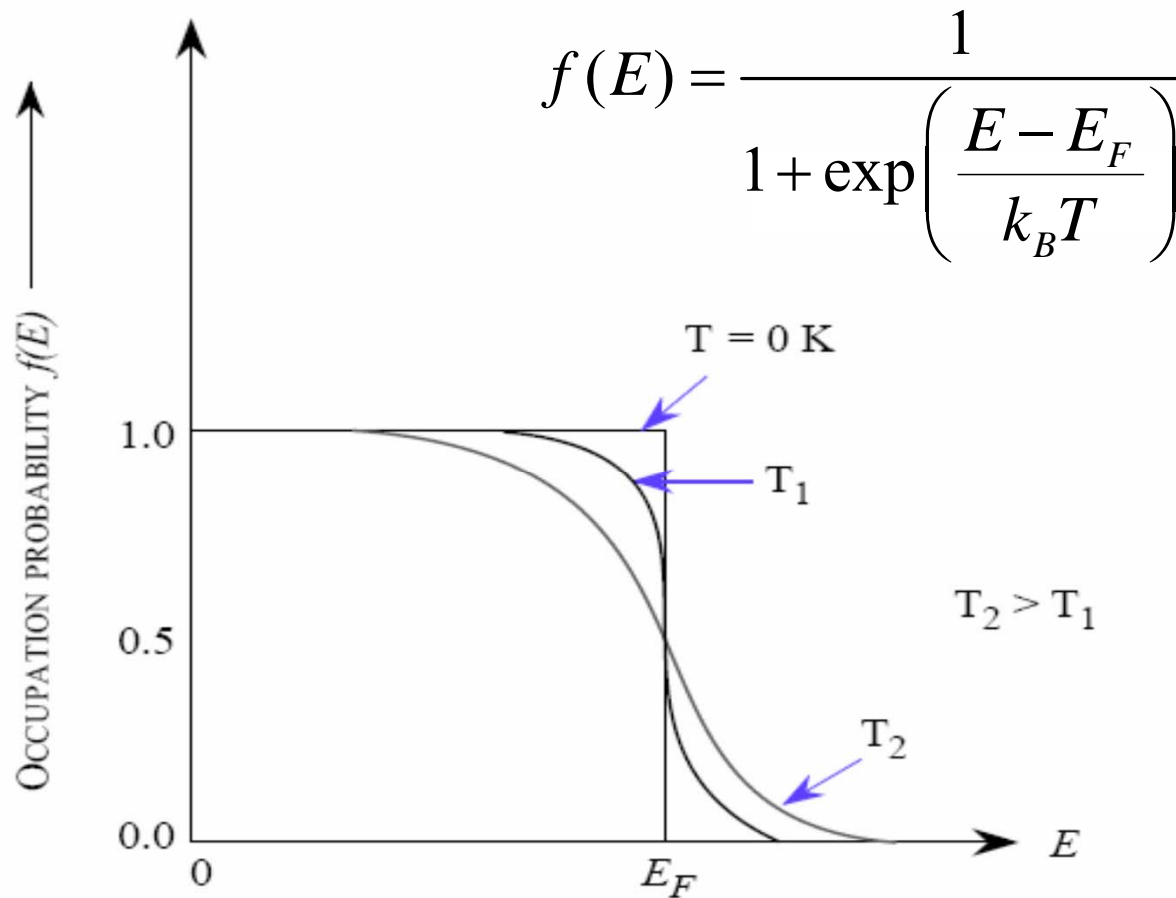
Si II,  $\beta$ -Sn, tetragonal

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

