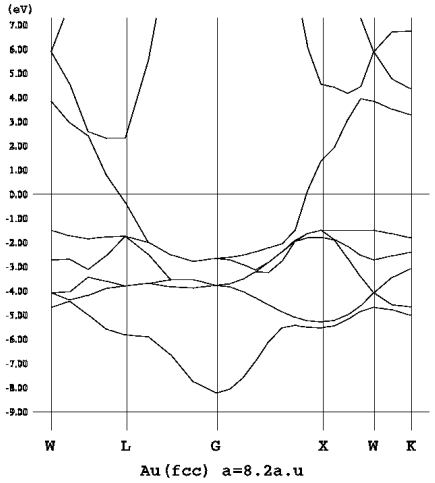
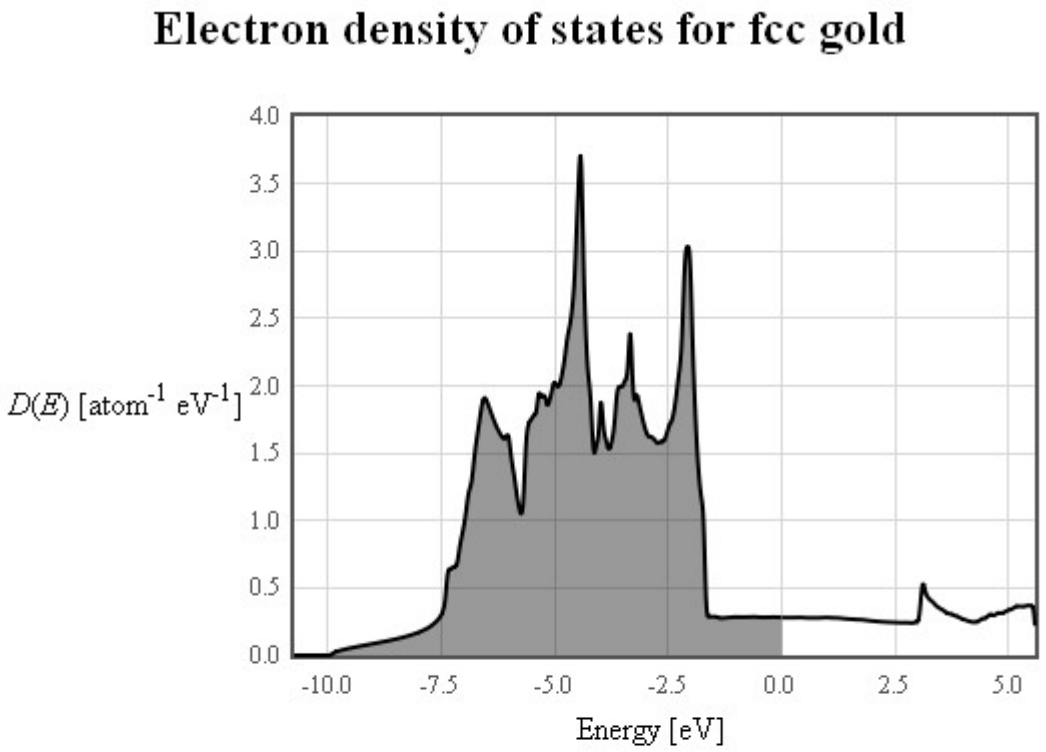
Electrons

Thermodynamic properties of metals

From the band structure measurements, we obtain the electron density of states.





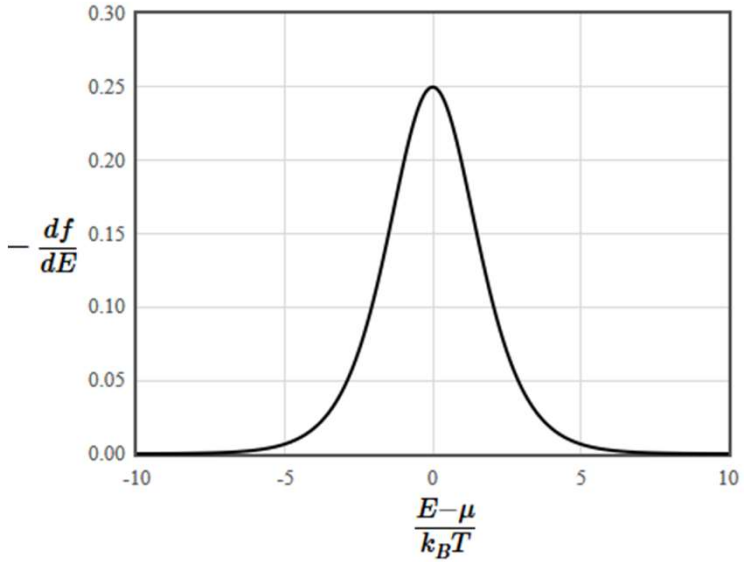
Thermodynamic properties can be calculated from the tabulated data for the density of states

E [eV]	$D(E)$ [atom^{-1} eV^{-1}]
-10.74913	0
-10.73552	0
-10.72192	0

Thermodynamic properties of metals

$$n = \int_{-\infty}^{\infty} D(E) f(E) dE, \qquad u = \int_{-\infty}^{\infty} E D(E) f(E) dE.$$

$$\int_{-\infty}^{\infty} H(E) f(E)\, dE$$



$$\int_{-\infty}^{\infty} H(E) f(E)\, dE = K(\infty) f(\infty) - K(-\infty) f(-\infty) - \int_{-\infty}^{\infty} K(E) \frac{df}{dE} dE,$$

$$f(E) = \frac{1}{\exp\left(\frac{E-\mu}{k_B T}\right) + 1}.$$

$$K(E) = \int_{-\infty}^{E} H(E')\, dE'$$

http://lampz.tugraz.at/~hadley/ss1/fermigas/sommerfeldtable/sommerfeld.php

Sommerfeld expansion for metals

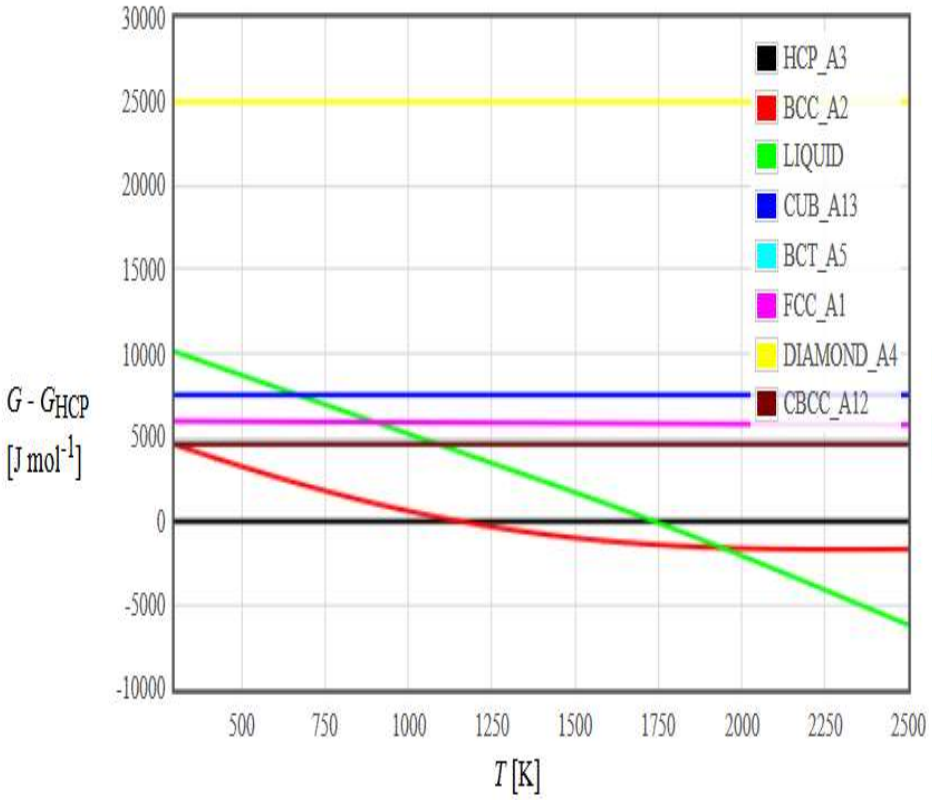
Chemical potential μ Implicitly defined by $n = \int_{-\infty}^{\infty} D(E) f(E) dE$	$\mu \approx E_F - \frac{\pi^2}{6}(k_B T)^2 \frac{D'(E_F)}{D(E_F)}$ [J]
Internal energy $u = \int_{-\infty}^{\infty} E D(E) f(E)\, dE$	$u \approx \int_{-\infty}^{E_F} E D(E) dE + \frac{\pi^2 D(E_F)}{6}(k_B T)^2$ [J m^{-3}]
Specific heat $c_v = \left(\frac{du}{dT}\right)_{V=\text{const}}$	$c_v \approx \frac{\pi^2 D(E_F)}{3} k_B^2 T$ [J m^{-3} K^{-1}]

Entropy $s = \int \frac{c_v}{T} dT$	$s \approx \frac{\pi^2 D(E_F)}{3} k_B^2 T$ [J m^{-3} K^{-1}]
Helmholtz free energy $f = u - Ts$	$f \approx \int_{-\infty}^{E_F} E D(E) dE - \frac{\pi^2 D(E_F)}{6}(k_B T)^2$ [J m^{-3}]

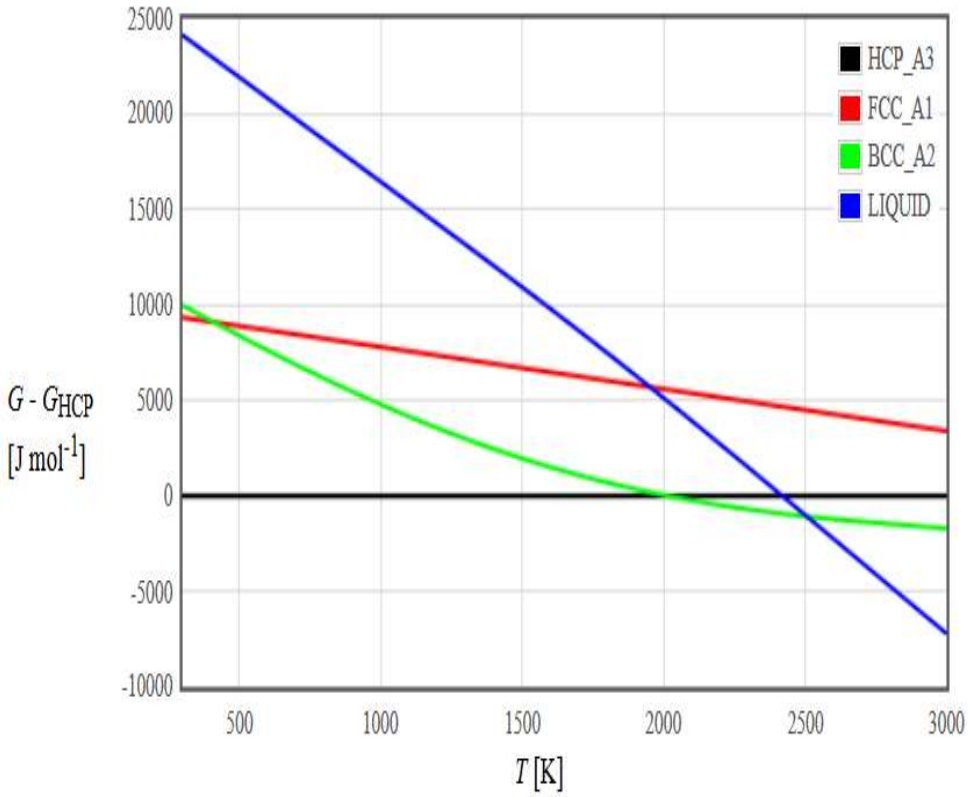
http://lampz.tugraz.at/~hadley/ss1/fermigas/sommerfeldtable/sommerfeld.php

Close packed → bcc

Ti



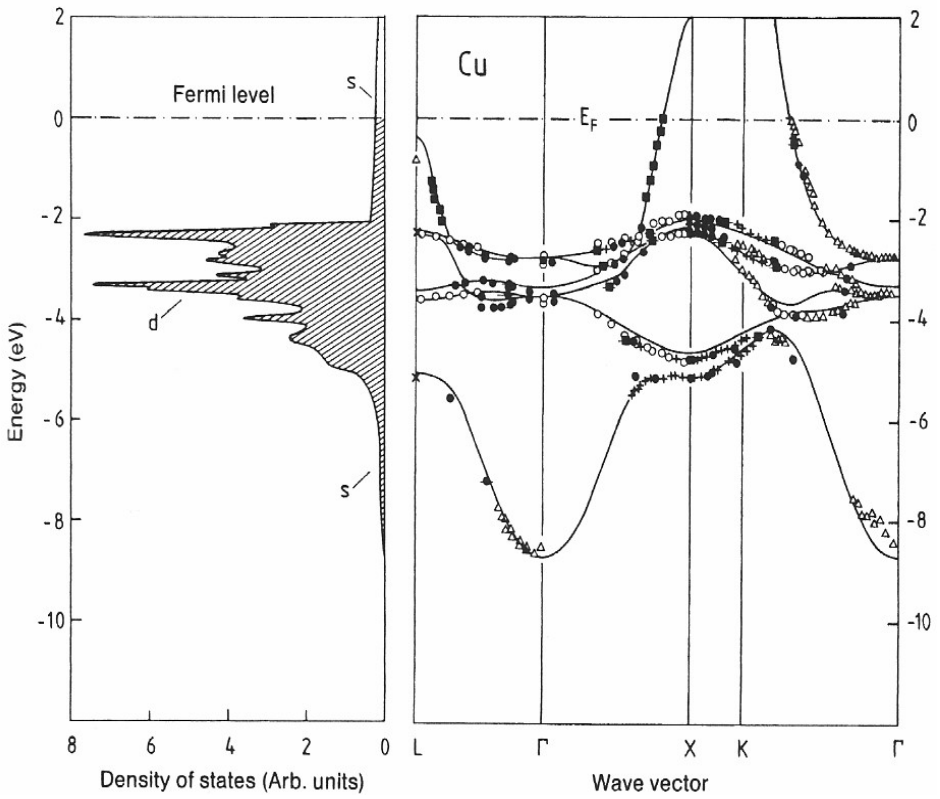
Hf

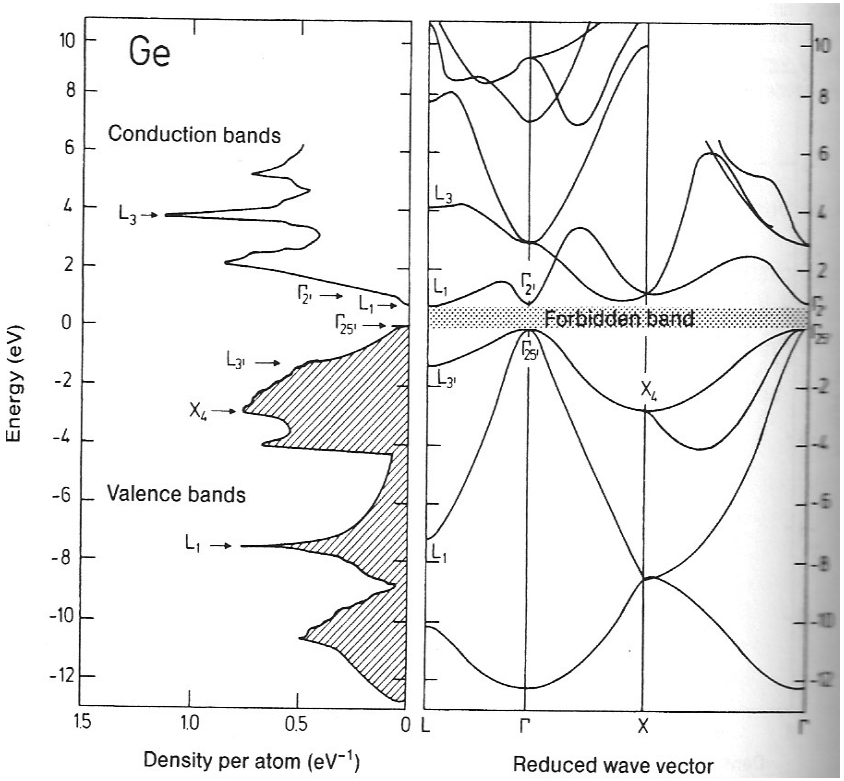


Close packed → bcc: Am, Be, Ca, Gd, Nd, Pr, Hf, Sc, Sm, Sr, Ti, Tb, Th, Tl, Y, Yb, Zr

http://lampx.tugraz.at/~hadley/ss1/materials/sgte/SGTE.html

Metals, semiconductors, and insulators



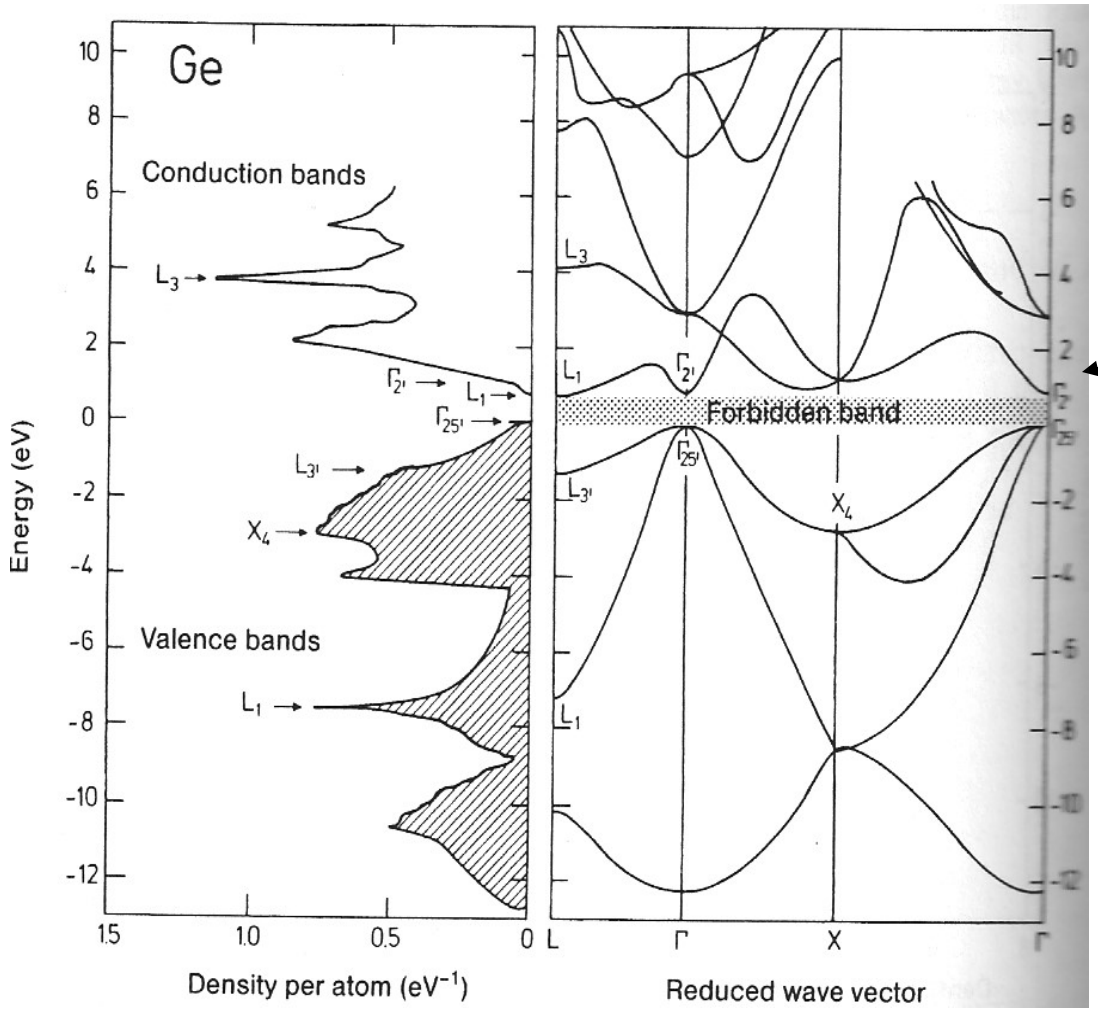


Insulators: band gap > 3 eV

From Ibach & Lueth

Semiconductors

Semiconductors



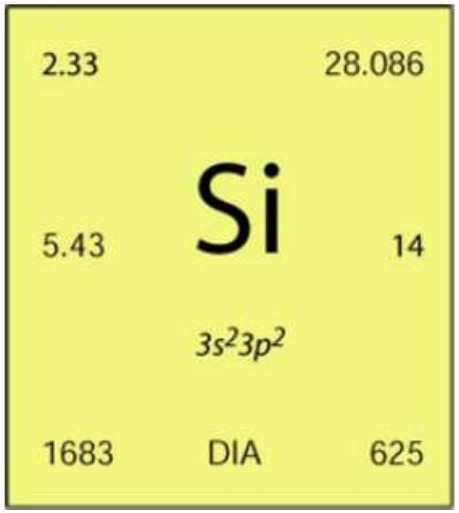
Conduction band

Valence band

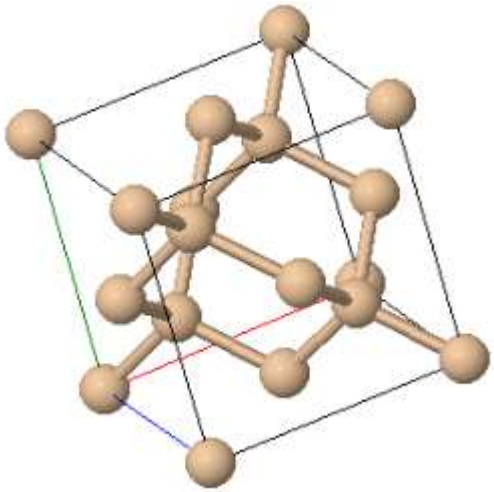
$$n = \int_{-\infty}^{\infty} D(E) f(E) dE$$

From Ibach & Lueth

Silicon



- Important semiconducting material
- 2nd most common element on earths crust (rocks, sand, glass, concrete)
- Often doped with other elements
- Oxide SiO_2 is a good insulator



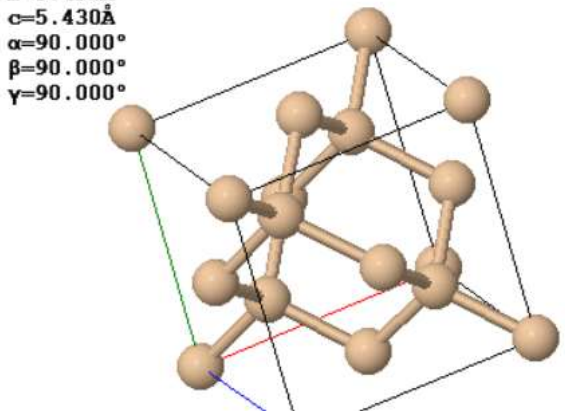
silicon crystal = diamond crystal structure

Silicon

Silicon is the second most common element in the earth's crust and an important semiconducting material.

Structural properties

Crystal structure: Diamond
Bravais lattice: face centered cubic
Space group: 227 (F d -3 m), Strukturbericht: A4, Pearson symbol: cF8
Point group: m3m (O_h) six 2-fold rotations, four 3-fold rotations, three 4-fold rotations, nine mirror planes, inversion
Lattice constant: $a = 0.543$ nm
Atomic weight 28.09
Atomic density $n_{atoms} = 4.995 \times 10^{22}$ 1/cm³
Density $\rho = 2.33$ g/cm³
Density of surface atoms
(100) 6.78×10^{14} 1/cm²
(110) 9.59×10^{14} 1/cm²
(111) 7.83×10^{14} 1/cm²

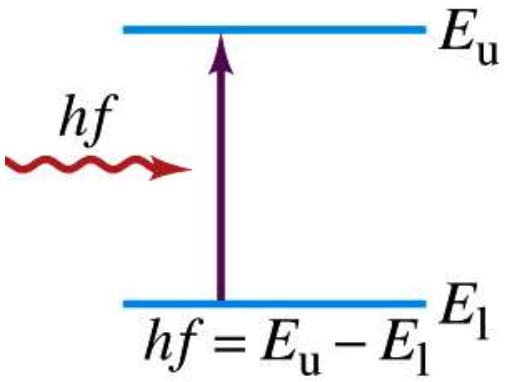


Conventional unit cell | Primitive unit cell | Asymmetric unit
2 x 2 x 2 | 3 x 3 x 3 | 5 x 5 x 5
Ball and Stick | Spacefill

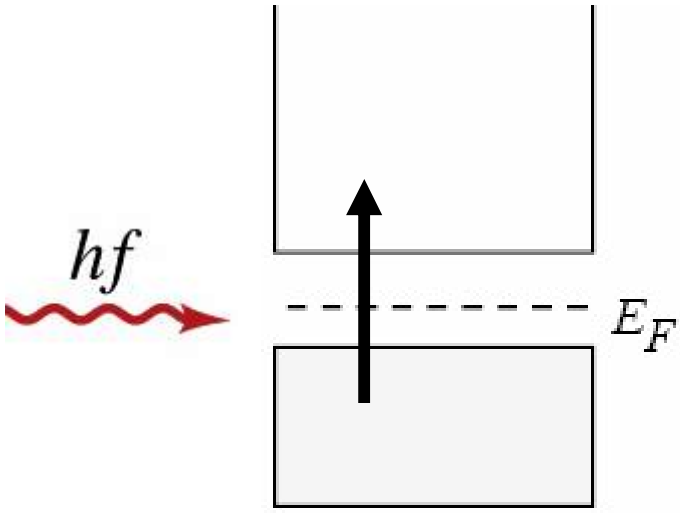
H: 1 K: 0 L: 0
show HKL plane | hide HKL plane
draw atoms in HKL plane
Thickness of HKL planes:

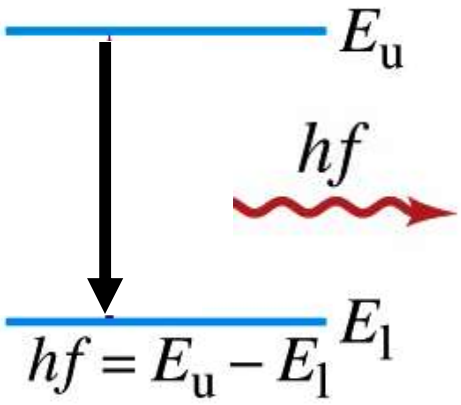
The conventional unit cell is a cube with sides of 0.543 nm. There are 8 atoms atoms in the conventional unit cell. (The

Absorption and emission of photons

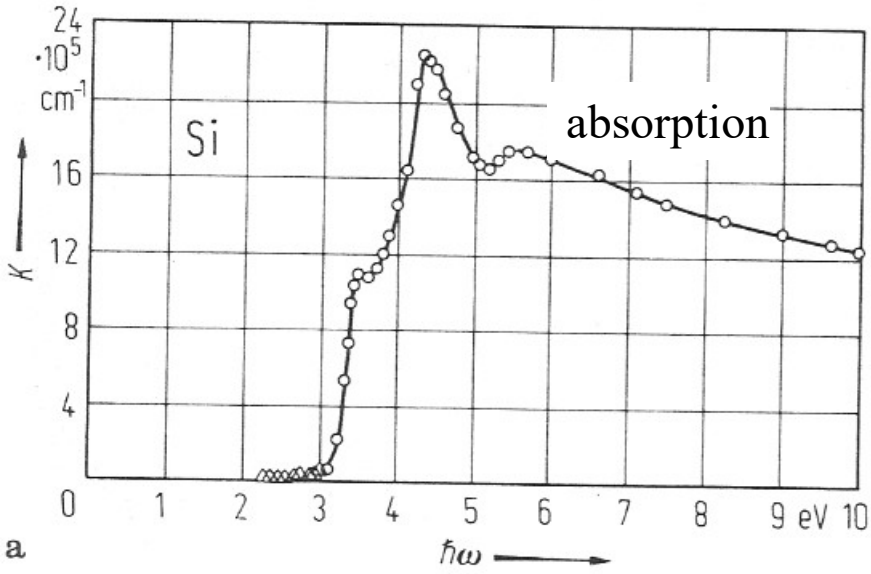


absorption

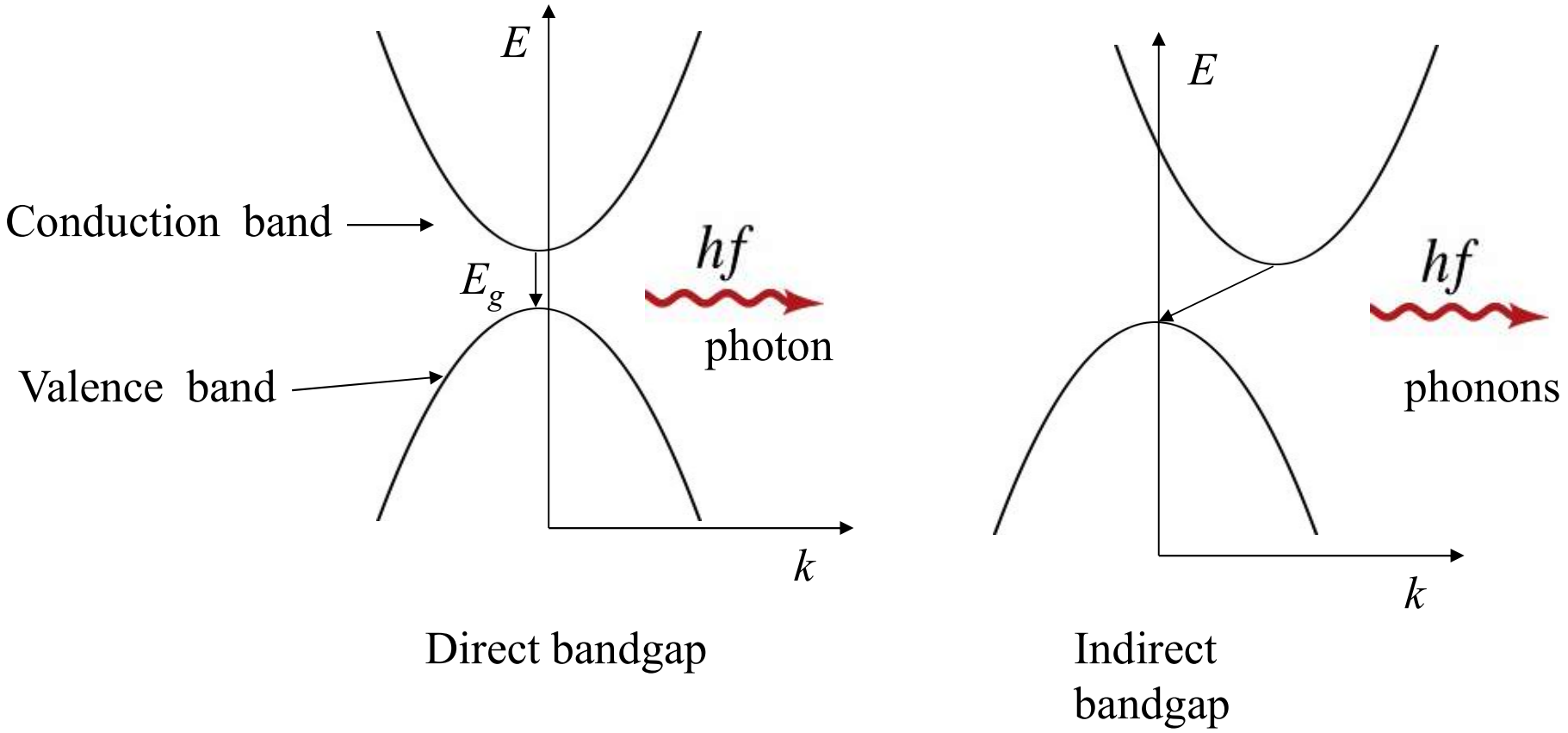




emission

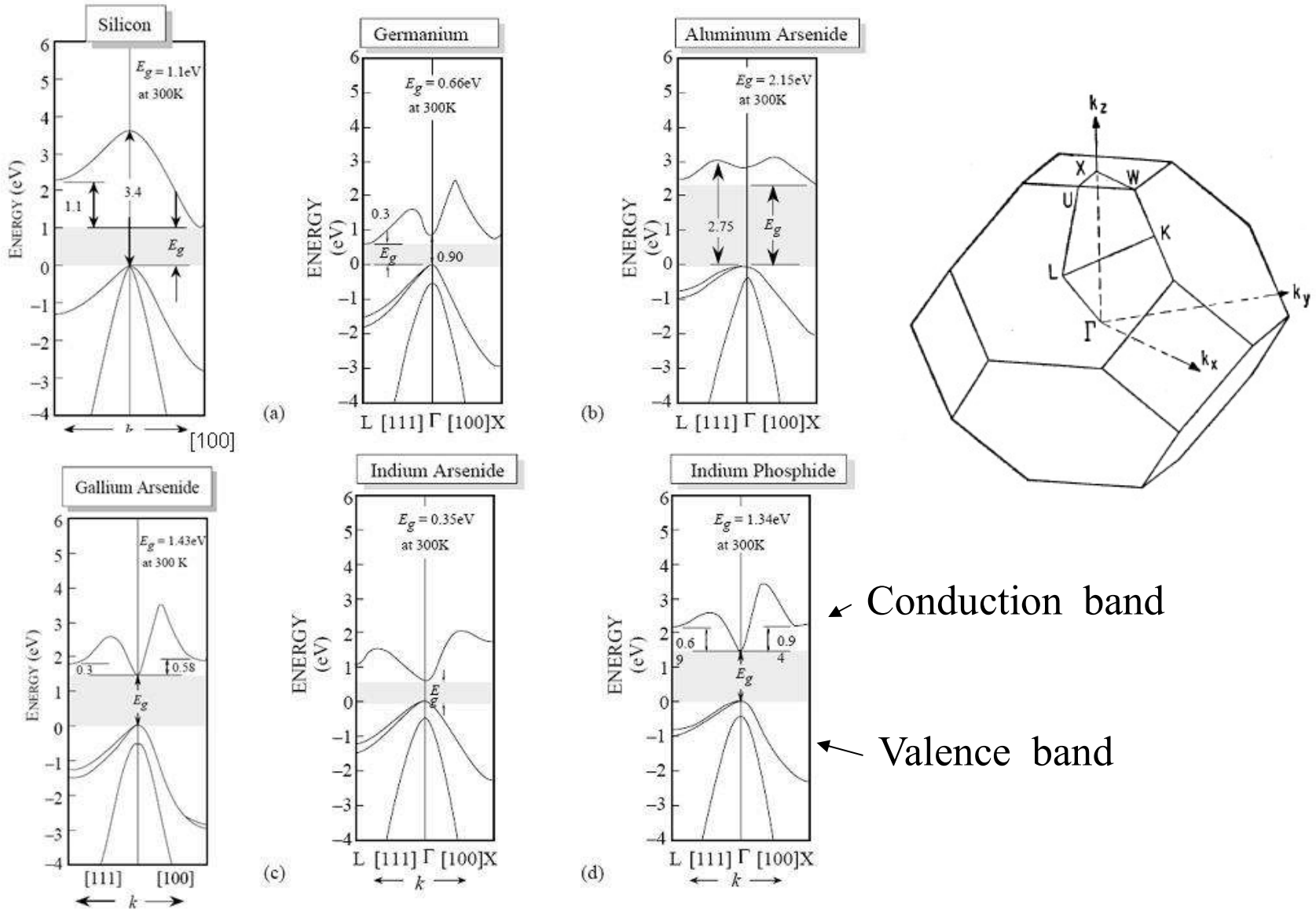


Direct and indirect band gaps



Direct bandgap semiconductors are used for optoelectronics

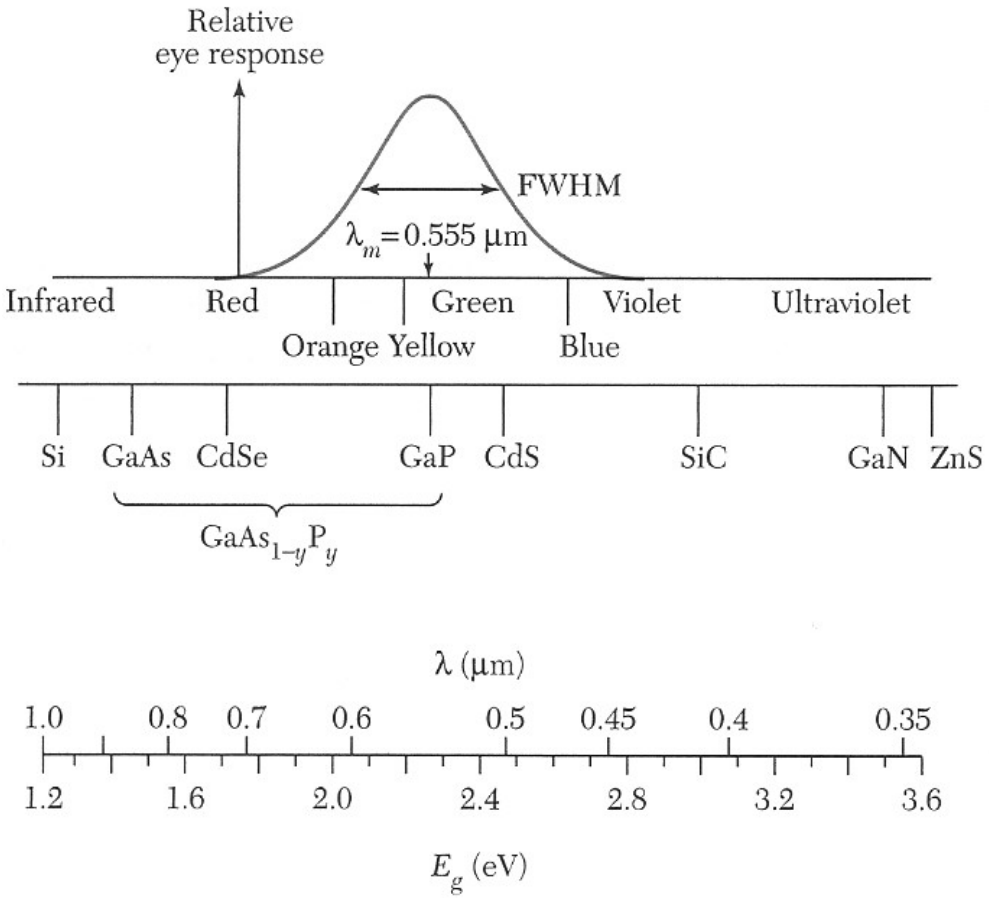
Semiconductors



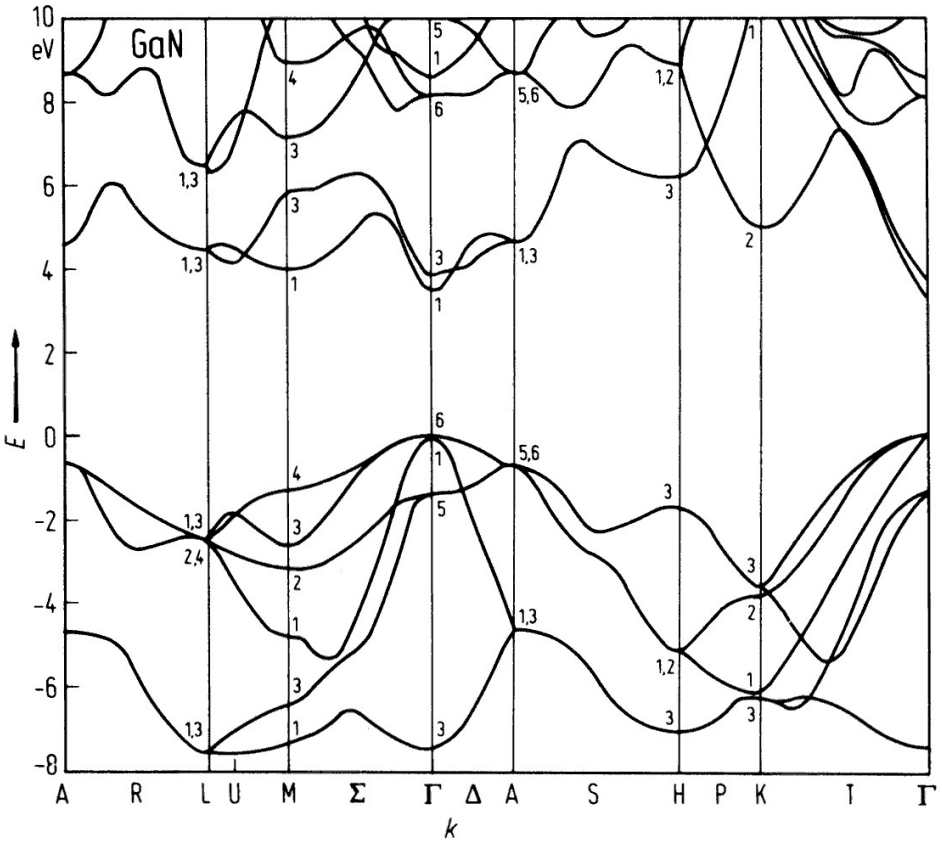
Light emitting diodes

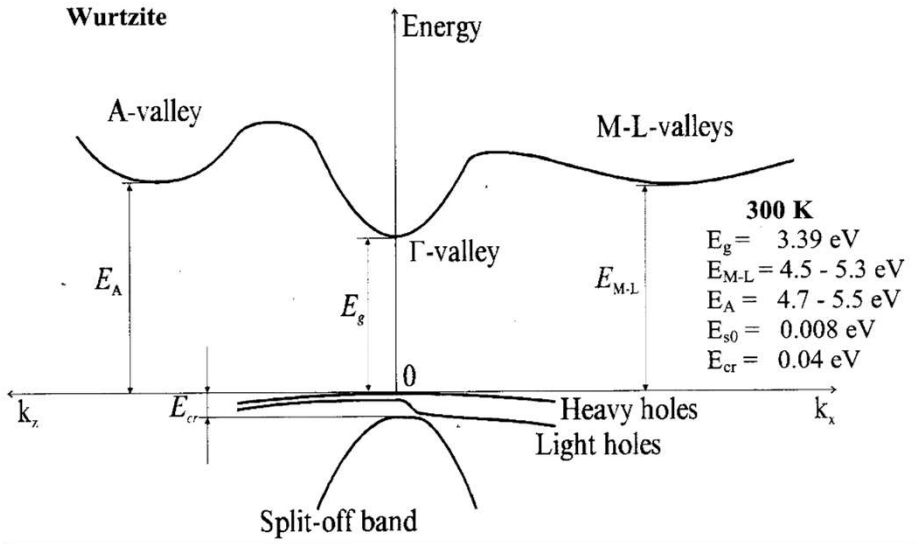
TABLE 1 Common III-V materials used to produce LEDs and their emission wavelengths.

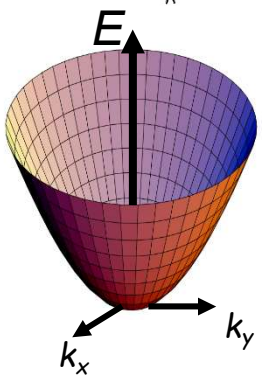
Material	Wavelength (nm)
InAsSbP/InAs	4200
InAs	3800
GaInAsP/GaSb	2000
GaSb	1800
$Ga_xIn_{1-x}As_{1-y}P_y$	1100-1600
$Ga_{0.47}In_{0.53}As$	1550
$Ga_{0.27}In_{0.73}As_{0.63}P_{0.37}$	1300
GaAs:Er,InP:Er	1540
Si:C	1300
GaAs:Yb,InP:Yb	1000
$Al_xGa_{1-x}As$:Si	650-940
GaAs:Si	940
$Al_{0.11}Ga_{0.89}As$:Si	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

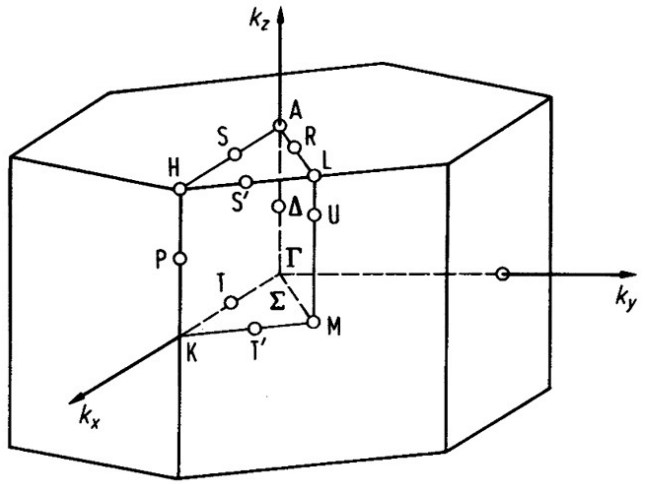


GaN





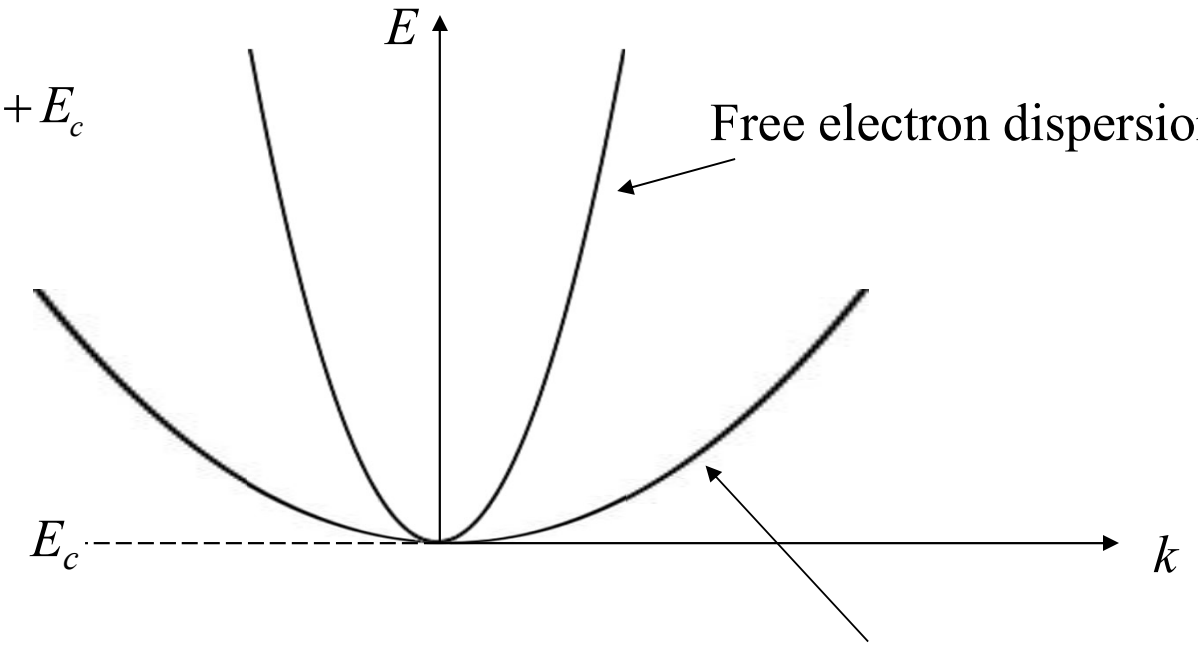




1st Brillioun zone of hcp

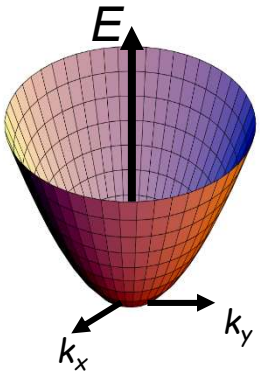
Conduction band minimum

$$E = \frac{\hbar^2 \left(\vec{k} - \vec{k}_0\right)^2}{2m^*} + E_c$$



Near the conduction band minimum, the bands are approximately parabolic.

Effective mass



$$E = \frac{\hbar^2 \left(\vec{k} - \vec{k}_0\right)^2}{2m^*} + E_c$$

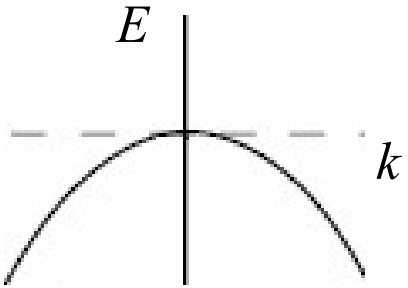
The parabola at the bottom of the conduction band does not have the same curvature as the free-electron dispersion relation. We define an effective mass to characterize the conduction band minimum.

$$m^* = \frac{\hbar^2}{\dfrac{d^2 E(\vec{k})}{dk_x^2}}$$

This effective mass is used to describe the response of electrons to external forces in the particle picture.

Top of the valence band

In the valence band, the effective mass is negative.



$$m^* = \frac{\hbar^2}{\frac{d^2E(\vec{k})}{dk_x^2}} < 0$$

Charge carriers in the valence band are positively charged holes.

$$m^*_h = \frac{-\hbar^2}{\frac{d^2E(\vec{k})}{dk_x^2}}$$

m^*_h = effective mass of holes

Holes

A completely filled band does not contribute to the current.

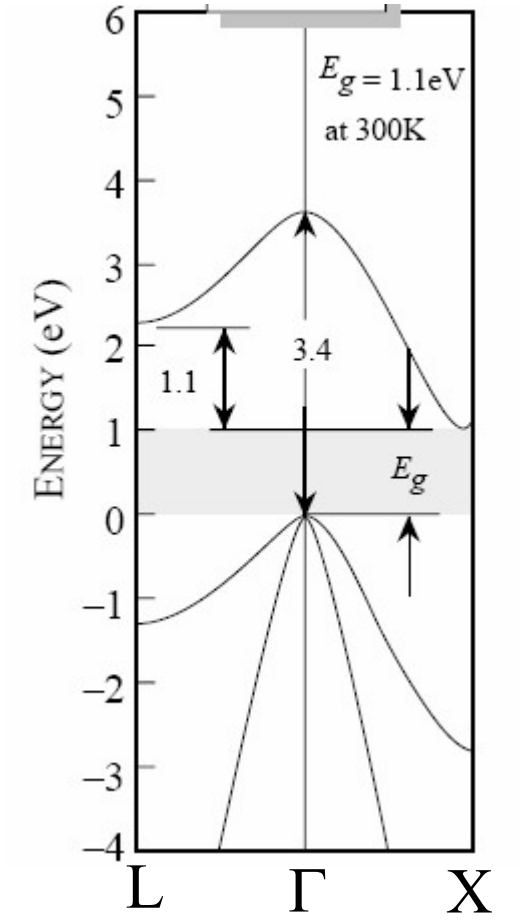
$$\vec{j} = \int_{\text{filled states}} -e\vec{v}(\vec{k})D(\vec{k})f(\vec{k})d\vec{k}$$

$$= \int_{\text{band}} -e\vec{v}(\vec{k})D(\vec{k})f(\vec{k})d\vec{k} - \int_{\text{empty states}} -e\vec{v}(\vec{k})D(\vec{k})f(\vec{k})d\vec{k}$$

$$= \int_{\text{empty states}} e\vec{v}(\vec{k})D(\vec{k})f(\vec{k})d\vec{k}$$

Holes have a positive charge and a positive mass.

Effective Mass



$$E = \frac{\hbar^2 \left(\vec{k} - \vec{k}_0\right)^2}{2m^*} + E_c$$

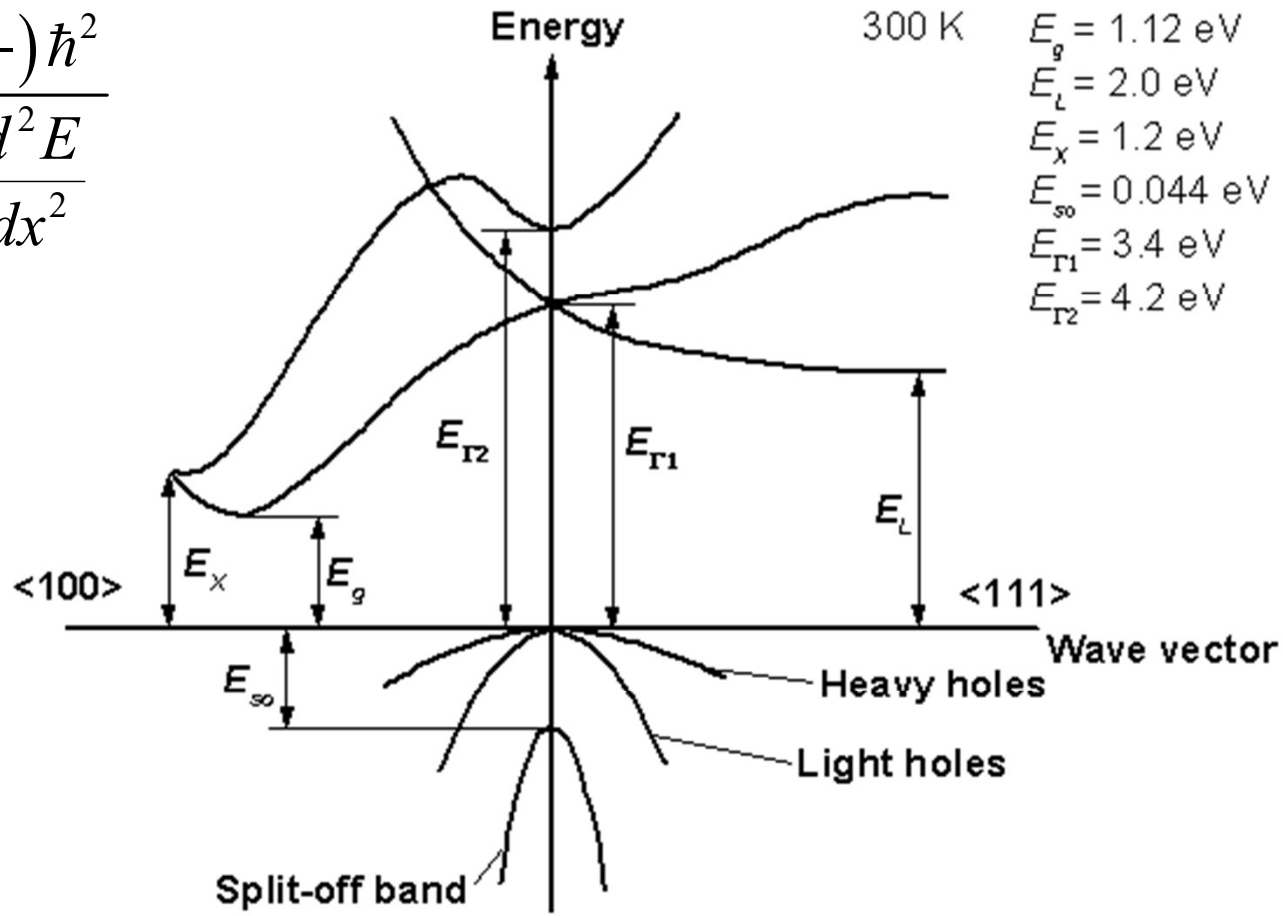
$$m_e^* = \frac{\hbar^2}{\frac{d^2E}{dk_x^2}}$$

$$E = \frac{-\hbar^2 \left(\vec{k} - \vec{k}_0\right)^2}{2m^*} + E_v$$

$$m_h^* = \frac{-\hbar^2}{\frac{d^2E}{dk_x^2}}$$

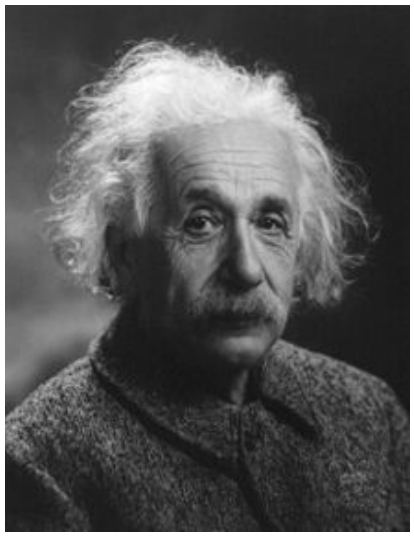
Silicon

$$m^*_{e,h} = \frac{(-)\hbar^2}{\frac{d^2E}{dx^2}}$$



http://www.matprop.ru/Si_bandstr#Basic

Holes

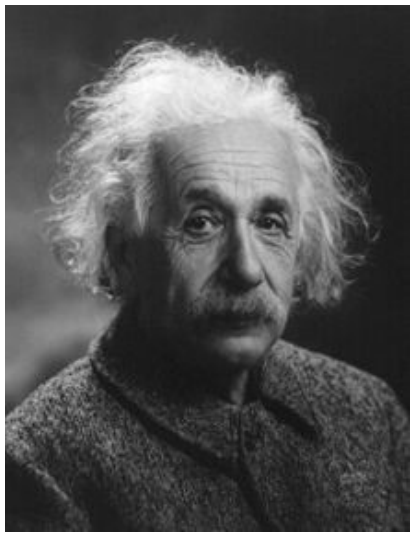


Albert Einstein

Erwin Schrödinger

Paul Adrien Maurice Dirac

Holes



Albert Einstein

Erwin Schrödinger

Paul Adrien Maurice Dirac

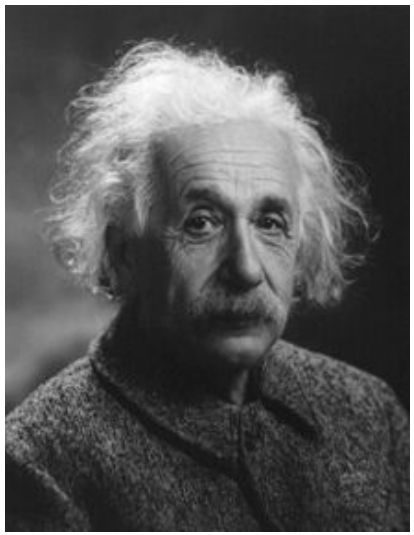
$$\frac{d^2u}{dt^2} = c^2 \frac{d^2u}{dx^2}$$

Wave equation

$$\frac{du}{dt} = k \frac{d^2u}{dx^2}$$

Heat equation

Holes



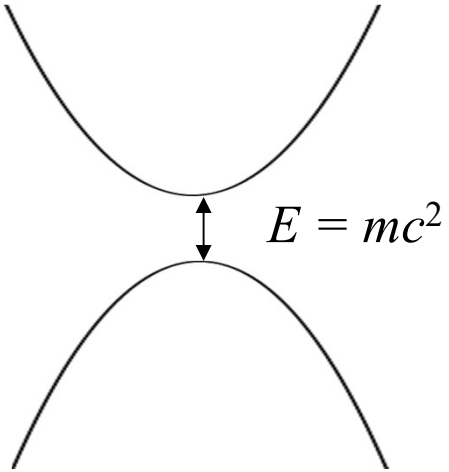
Albert Einstein

Erwin Schrödinger

Paul Adrien Maurice Dirac

$$\left(\beta mc^2 + \sum_{j=1}^{3} \alpha_j p_j c\right)\psi = i\hbar\frac{\partial\psi}{\partial t}$$

Dirac equation

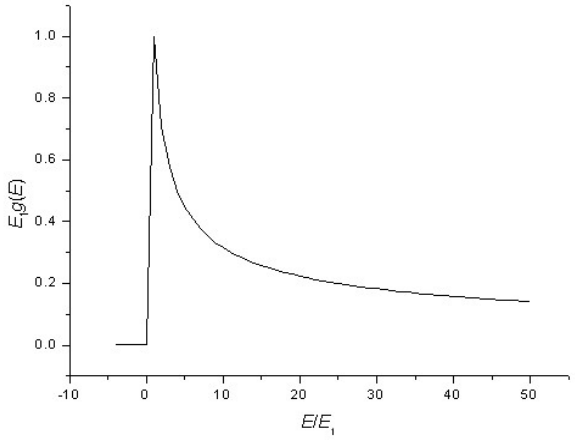


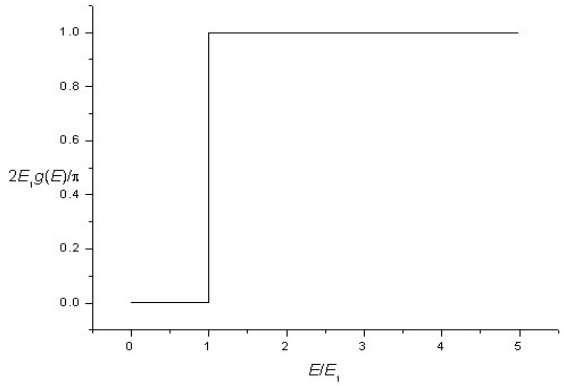
Free electron Fermi gas

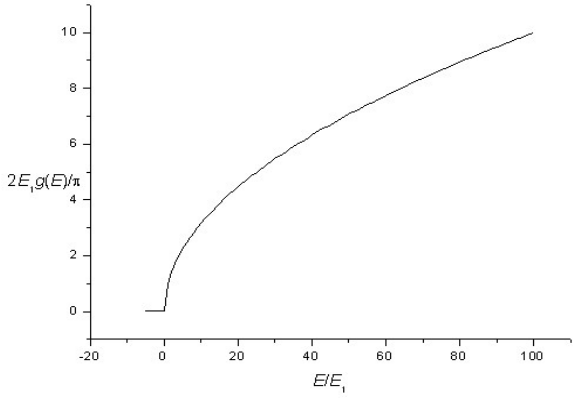
1 - d $$D(E) = \sqrt{\frac{2m}{\hbar^2 \pi^2 E}} = \frac{n}{2\sqrt{E_F E}} \qquad \mathrm{J^{-1}m^{-1}}$$

2 - d $$D(E) = \frac{m}{\hbar^2 \pi} = \frac{n}{E_F} \qquad \mathrm{J^{-1}m^{-2}}$$

3 - d $$D(E) = \frac{\pi}{2}\left(\frac{2m}{\hbar^2 \pi^2}\right)^{3/2} \sqrt{E} = \frac{3n}{2E_F^{3/2}} \sqrt{E} \qquad \mathrm{J^{-1}m^{-3}}$$



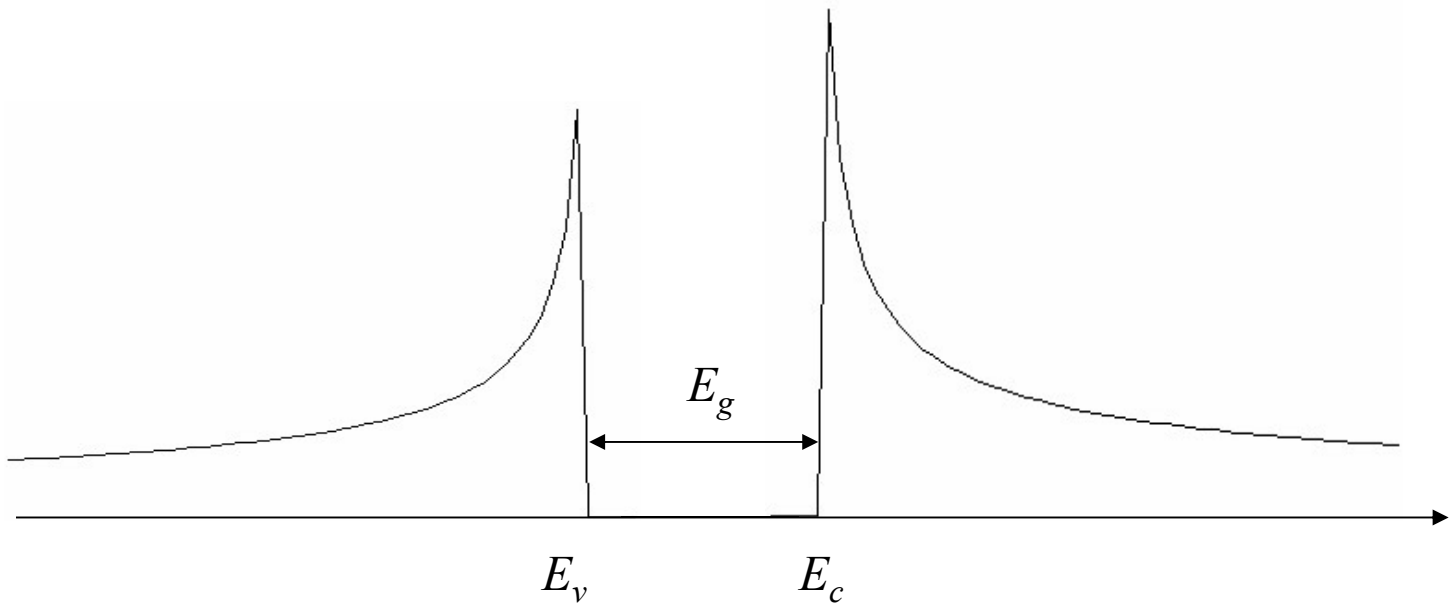




Semiconductors and insulators - 1d

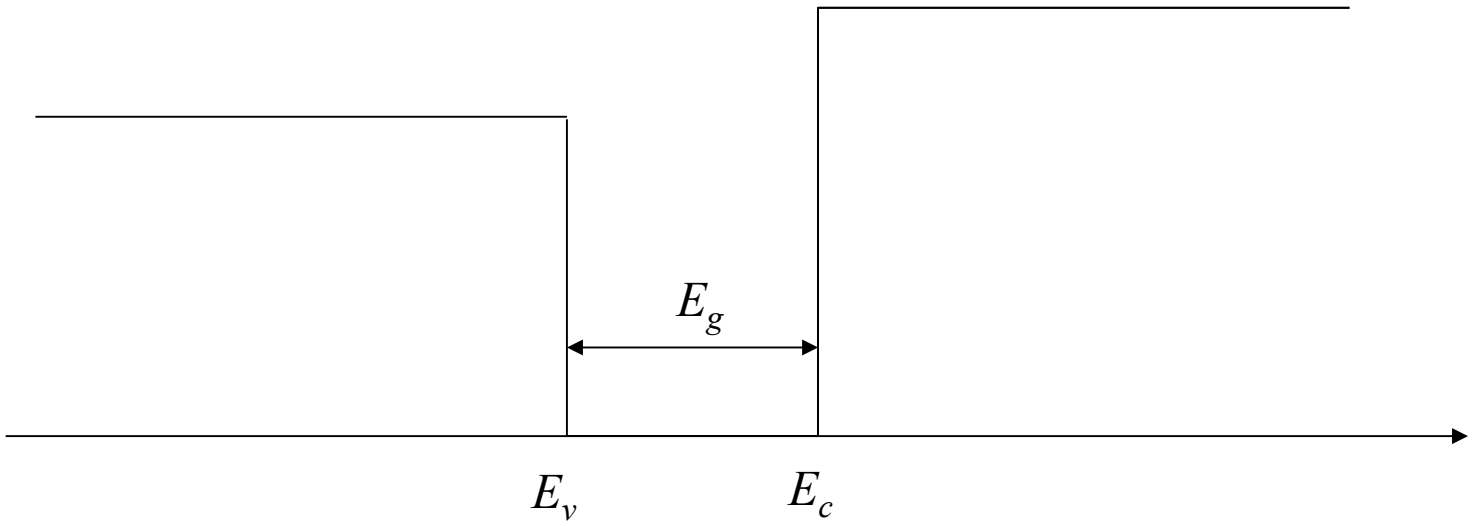
$$E = \frac{\hbar^2 (\vec{k} - \vec{k}_0)^2}{2m^*}$$

$$D(E) = \begin{cases} \dfrac{D_c}{\sqrt{(E_v - E)}} & E < E_v \\ 0 & E_v < E < E_c \\ \dfrac{D_v}{\sqrt{(E - E_c)}} & E_c < E \end{cases} \quad \mathrm{J^{-1}m^{-3}}$$



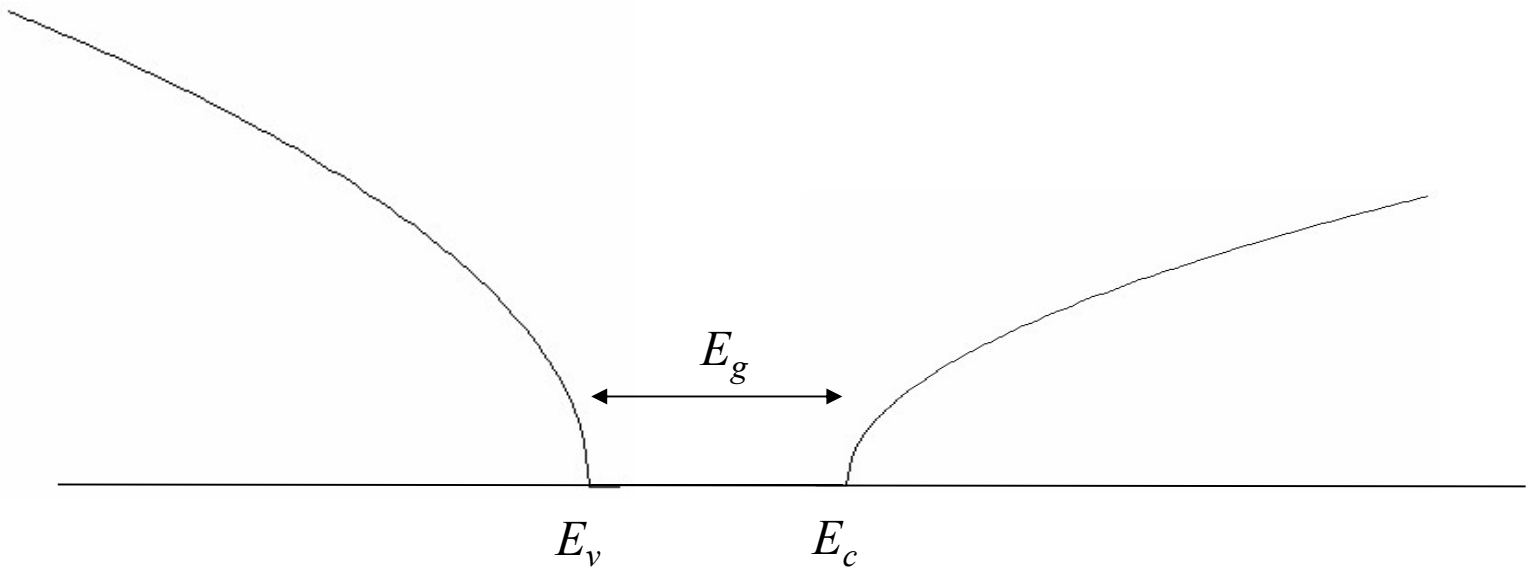
Semiconductors and insulators - 2d

$$D(E) = \begin{cases} D_c & E < E_v \\ 0 & E_v < E < E_c \\ D_v & E_c < E \end{cases} \quad \mathrm{J^{-1}m^{-3}}$$



Semiconductors and insulators - 3d

$$D(E) = \begin{cases} D_c \sqrt{E_v - E} & E < E_v \\ 0 & E_v < E < E_c \\ D_v \sqrt{E - E_c} & E_c < E \end{cases} \quad \mathrm{J^{-1}m^{-3}}$$



Silicon density of states