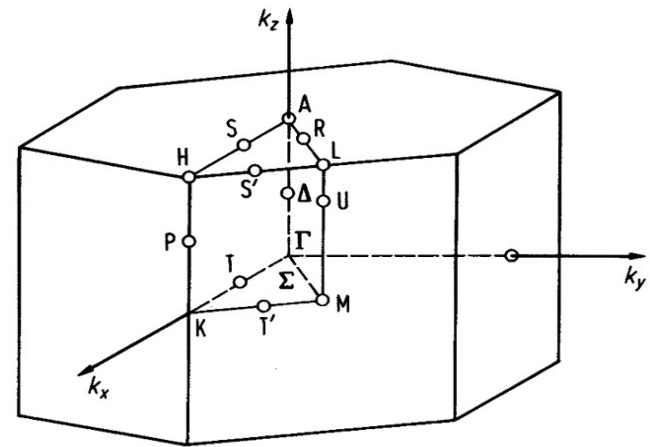
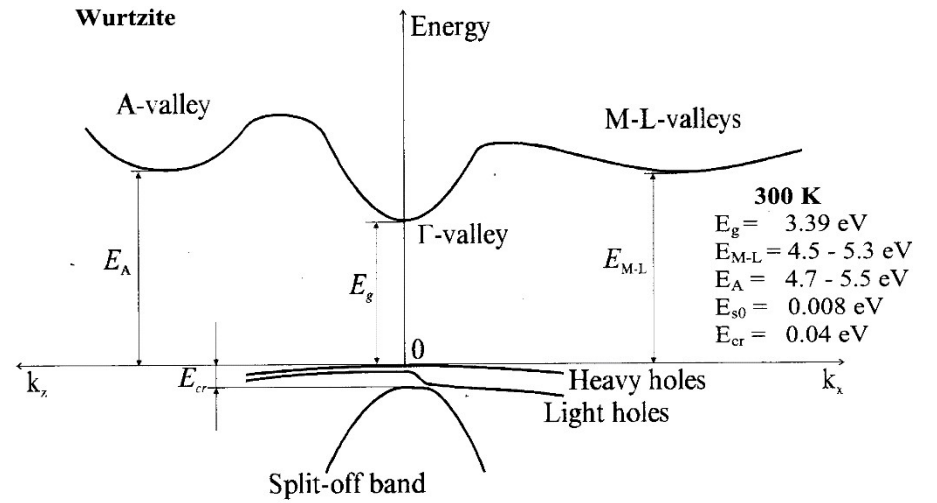
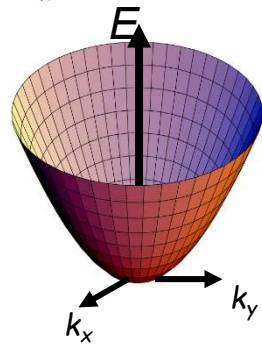
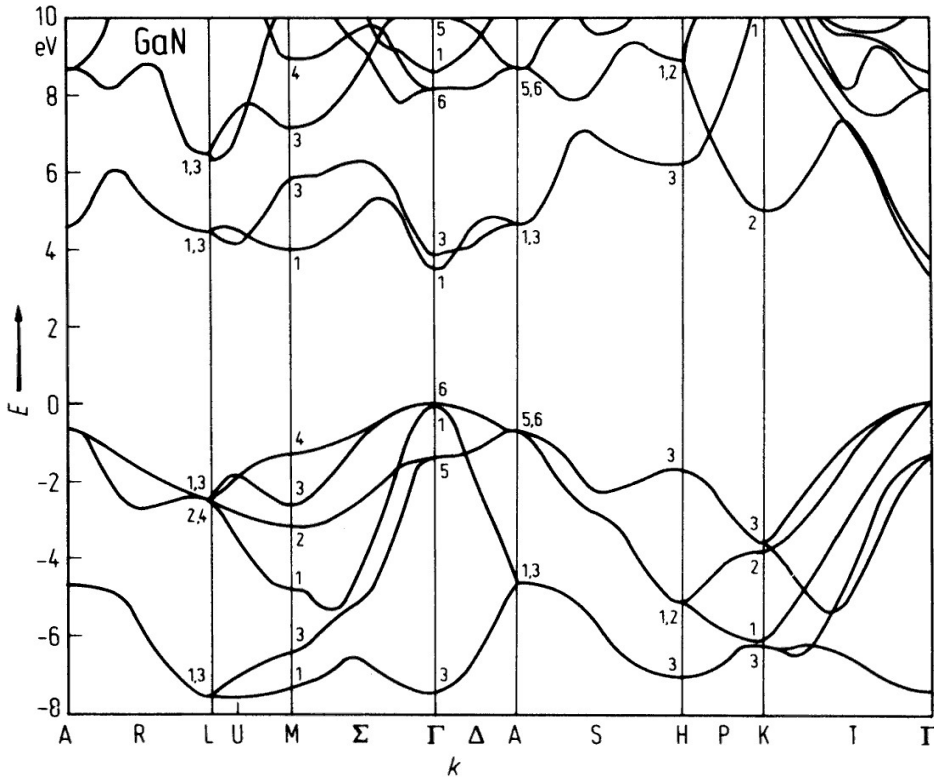


# GaN



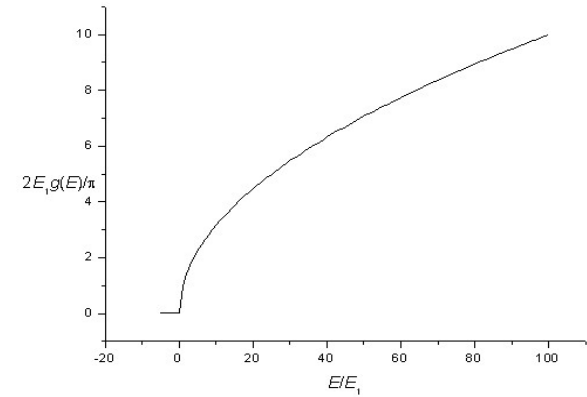
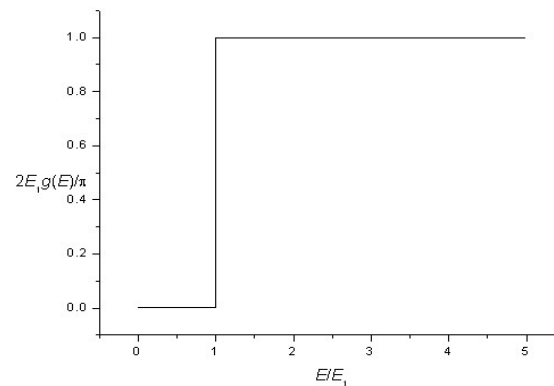
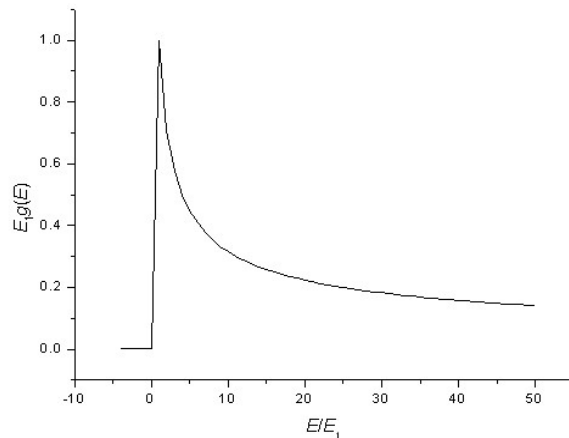
1st Brillouin zone of hcp

# Free electron Fermi gas

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

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

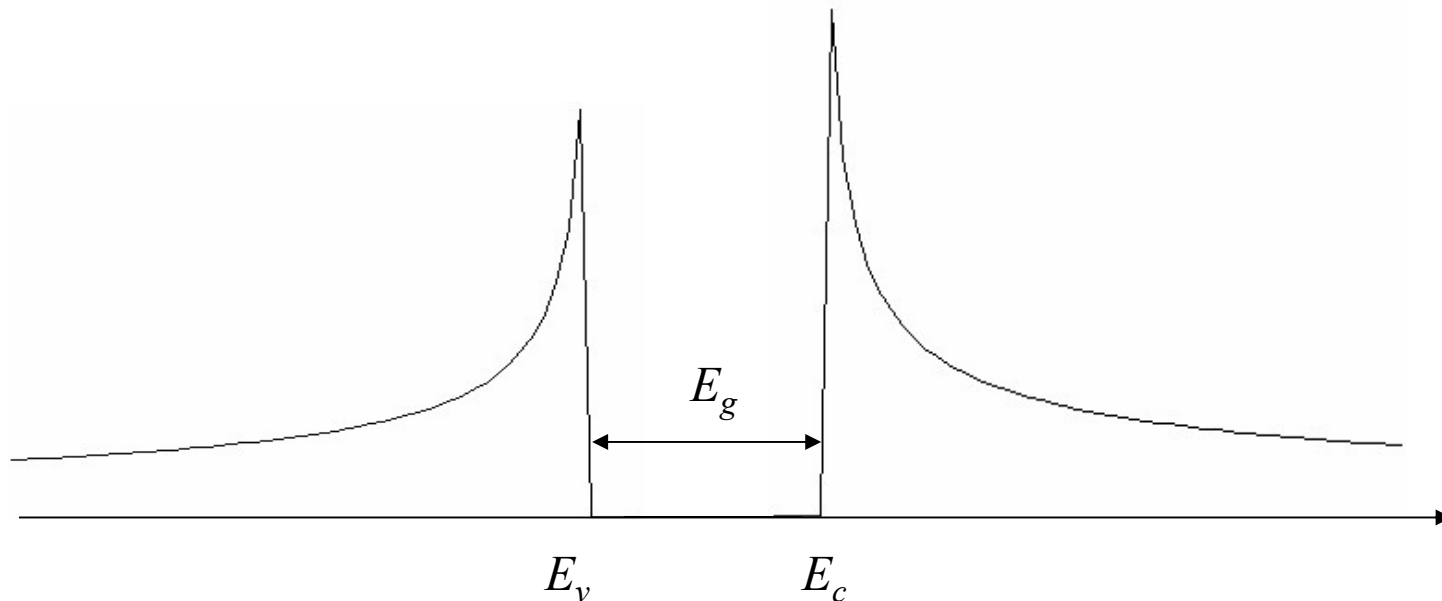
3 - d  $D(E) = \frac{\pi}{2} \left( \frac{2m}{\hbar^2 \pi^2} \right)^{3/2} \sqrt{E} = \frac{3n}{2E_F^{3/2}} \sqrt{E} \quad \text{J}^{-1} \text{m}^{-3}$



# Semiconductors and insulators - 1d

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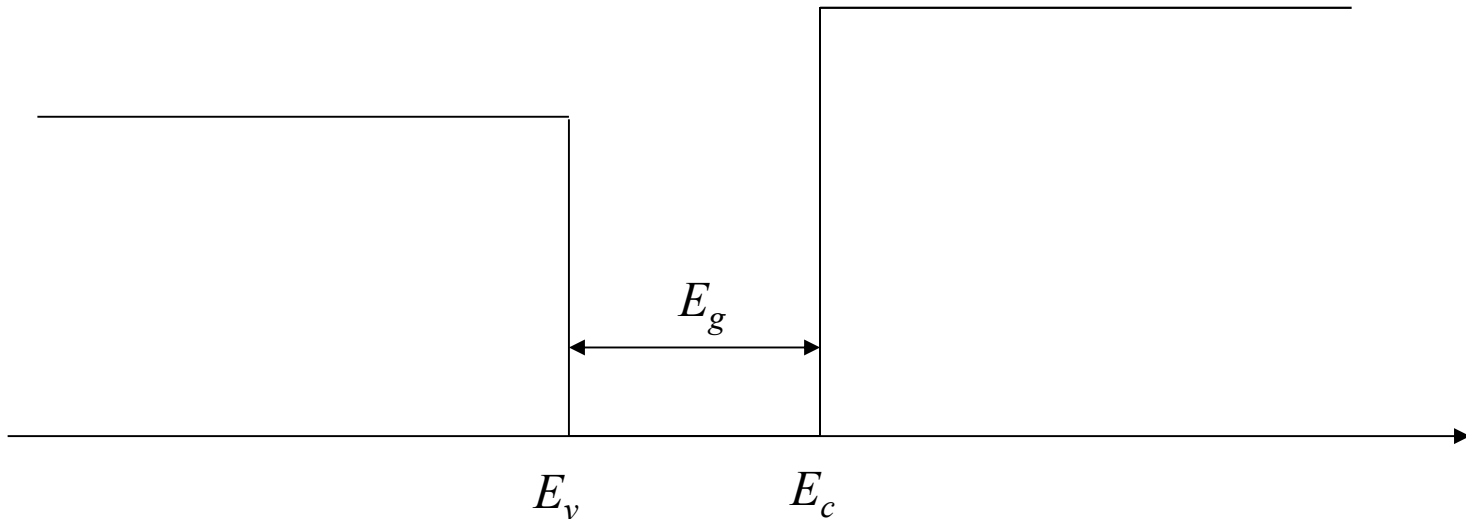
$$E = \frac{\hbar^2 (\vec{k} - \vec{k}_0)^2}{2m^*}$$
$$D(E) = \begin{cases} \sqrt{\frac{2m_h^*}{\hbar^2 \pi^2 (E_v - E)}} & E < E_v \\ 0 & E_v < E < E_c \\ \sqrt{\frac{2m_e^*}{\hbar^2 \pi^2 (E - E_c)}} & E_c < E \end{cases} \quad \text{J}^{-1} \text{m}^{-3}$$



# Semiconductors and insulators - 2d

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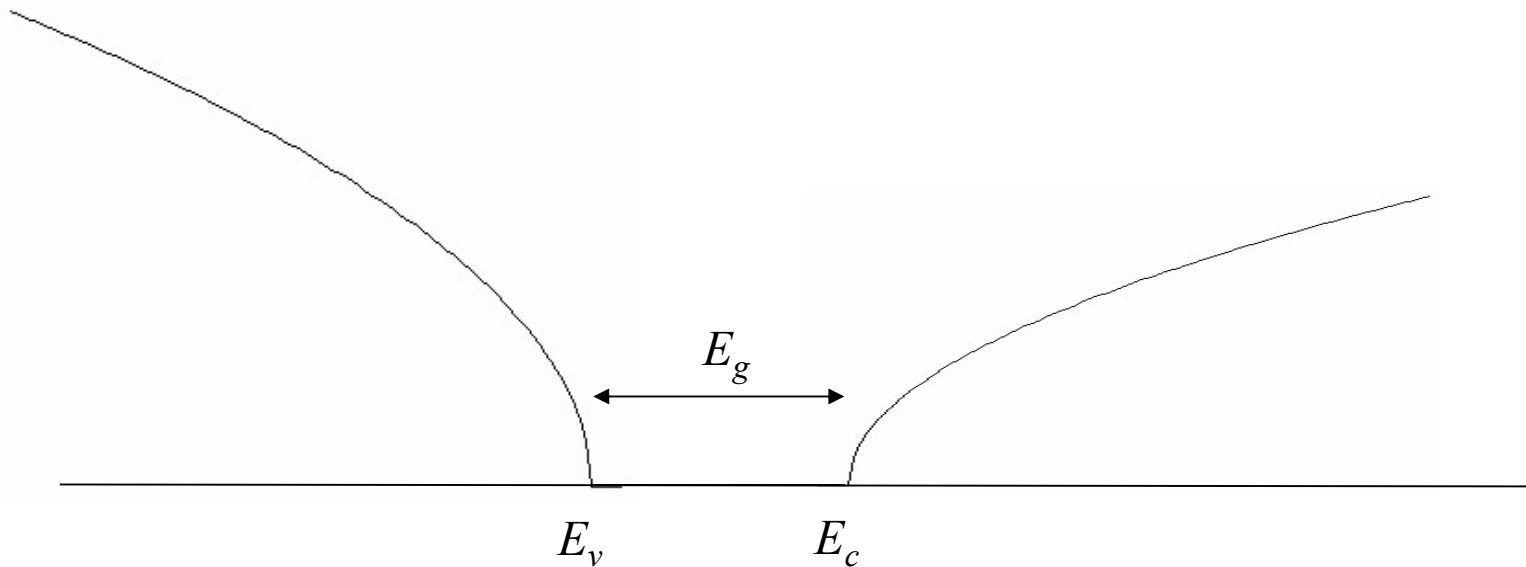
$$D(E) = \begin{cases} \frac{m_h^*}{\hbar^2 \pi} & E < E_v \\ 0 & E_v < E < E_c \\ \frac{m_e^*}{\hbar^2 \pi} & E_c < E \end{cases} \quad \text{J}^{-1}\text{m}^{-3}$$



# Semiconductors and insulators - 3d

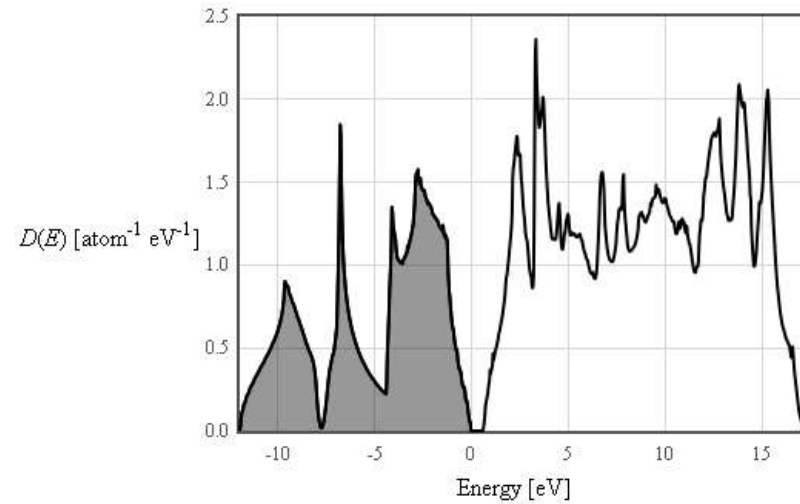
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$$D(E) = \begin{cases} \frac{(2m_h^*)^{\frac{3}{2}}}{2\pi^2 \hbar^3} \sqrt{E_v - E} & E < E_v \\ 0 & E_v < E < E_c \\ \frac{(2m_e^*)^{\frac{3}{2}}}{2\pi^2 \hbar^3} \sqrt{E - E_c} & E_c < E \end{cases} \quad \text{J}^{-1}\text{m}^{-3}$$

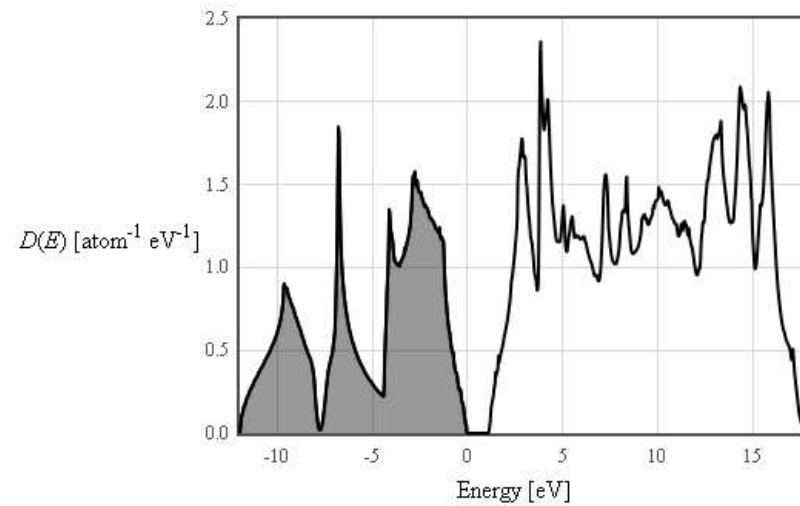


## Electron density of states for silicon

The density of states for silicon was calculated using the program [Quantum Espresso](#) (version 4.3.1). Notice that the bandgap is too small. This commonly occurs for semiconductors when the bandstructure is calculated with density functional theory. [Another calculation that uses wien2K](#).



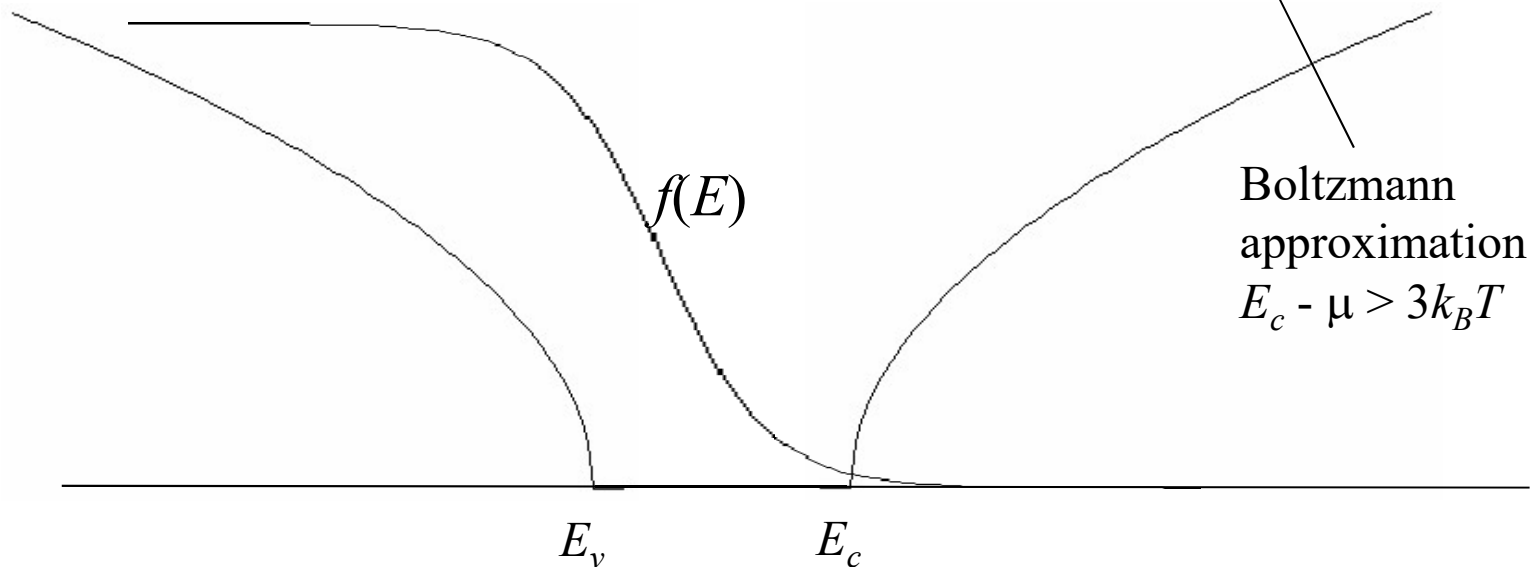
The common way to fix the small bandgap problem is simply to increase the energies of the states in the conduction band until the bandgap is the right size. This is sometimes known as a scissors operation. The density of states is cut in the bandgap and pushed apart until the bandgap is correct. The density of states after this correction has been performed is shown below.



# Density of electrons in the conduction band

The free electron density of states is modified by the effective mass.

$$D(E) = \frac{\pi}{2} \left( \frac{2m^*}{\hbar^2 \pi^2} \right)^{3/2} \sqrt{E - E_c} \quad f(E) = \frac{1}{1 + \exp\left(\frac{E - \mu}{k_B T}\right)} \approx \exp\left(\frac{\mu - E}{k_B T}\right)$$



$$n = \int_{E_c}^{\infty} D(E) f(E) dE \approx \frac{\pi}{2} \left( \frac{2m^*}{\hbar^2 \pi^2} \right)^{3/2} \int_{E_c}^{\infty} \exp\left(\frac{\mu - E}{k_B T}\right) \sqrt{E - E_c} dE$$

# Density of electrons in the conduction band

---

$$n = \int_{E_c}^{\infty} D(E) f(E) dE \approx \frac{\pi}{2} \left( \frac{2m^*}{\hbar^2 \pi^2} \right)^{3/2} \int_{E_c}^{\infty} \exp\left(\frac{\mu - E}{k_B T}\right) \sqrt{E - E_c} dE$$

$$\frac{\sqrt{\pi}}{2} = \int_0^{\infty} \sqrt{x} e^{-x} dx$$

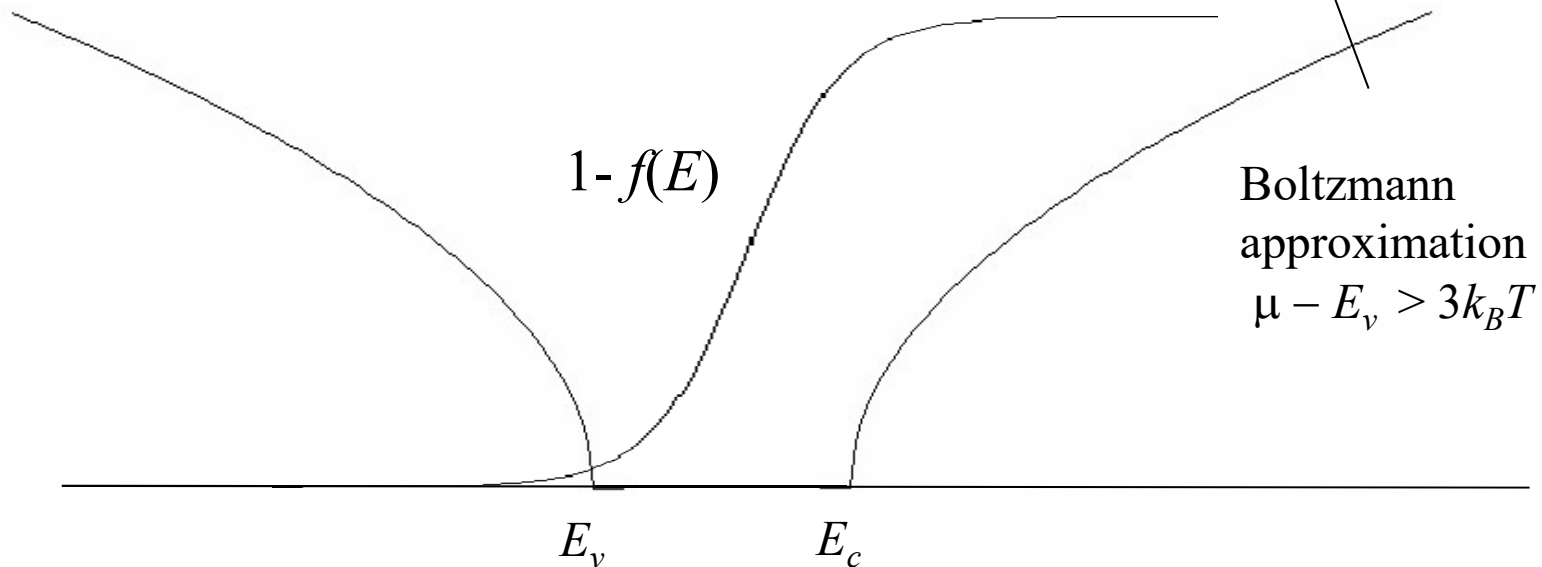
$$n = N_c \exp\left(\frac{\mu - E_c}{k_B T}\right)$$

$$N_c = 2 \left( \frac{m^* k_B T}{2\pi \hbar^2} \right)^{3/2} = \text{effective density of states}$$



# Density of holes in the valence band

$$D(E) = \frac{\pi}{2} \left( \frac{2m_h^*}{\hbar^2 \pi^2} \right)^{3/2} \sqrt{E_v - E} \quad 1 - f(E) = 1 - \frac{1}{1 + \exp\left(\frac{E - \mu}{k_B T}\right)} \approx \exp\left(\frac{E - \mu}{k_B T}\right)$$



$$p = \int_{-\infty}^{E_v} D(E)(1 - f(E)) dE \approx \frac{\pi}{2} \left( \frac{2m_h^*}{\hbar^2 \pi^2} \right)^{3/2} \int_{-\infty}^{E_v} \exp\left(\frac{E - \mu}{k_B T}\right) \sqrt{E_v - E} dE$$

# Density of holes in the valence band

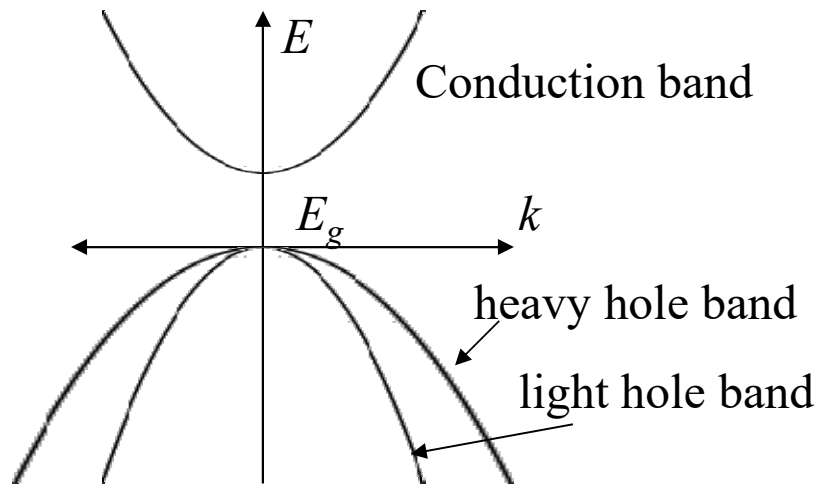
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$$p = \frac{1}{L^3} \int_{-\infty}^{E_v} N(E)(1 - f(E)) dE \approx \frac{\pi}{2} \left( \frac{2m_h^*}{\hbar^2 \pi^2} \right)^{3/2} \int_{-\infty}^{E_v} \exp\left(\frac{E - \mu}{k_B T}\right) \sqrt{E_v - E} dE$$

$$p = N_v \exp\left(\frac{E_v - \mu}{k_B T}\right)$$

$$N_v = 2 \left( \frac{m_h^* k_B T}{2\pi \hbar^2} \right)^{3/2} \quad = \text{Effective density of states in the valence band}$$

# Semiconductors



$$n = N_{c300} \left( \frac{T}{300} \right)^{3/2} \exp \left( \frac{\mu - E_c}{k_B T} \right)$$

$$p = N_{v300} \left( \frac{T}{300} \right)^{3/2} \exp \left( \frac{E_v - \mu}{k_B T} \right)$$

Properties	Si	Ge	GaAs
Bandgap $E_g$	1.12 eV	0.66 eV	1.424 eV
Effective density of states in conduction band (300 K) $N_c$	$2.78 \times 10^{25} \text{ m}^{-3}$	$1.04 \times 10^{25} \text{ m}^{-3}$	$4.45 \times 10^{23} \text{ m}^{-3}$
Effective density of states in valence band (300 K) $N_v$	$9.84 \times 10^{24} \text{ m}^{-3}$	$6.0 \times 10^{24} \text{ m}^{-3}$	$7.72 \times 10^{24} \text{ m}^{-3}$
Effective mass electrons $m^*/m_0$	$m_l^* = 0.98$ $m_t^* = 0.19$	$m_l^* = 1.64$ $m_t^* = 0.082$	$m^* = 0.067$
Effective mass holes $m^*/m_0$	$m_{lh}^* = 0.16$ $m_{hh}^* = 0.49$	$m_{lh}^* = 0.044$ $m_{hh}^* = 0.28$	$m_{lh}^* = 0.082$ $m_{hh}^* = 0.45$
Crystal structure	diamond	diamond	zincblende
Density	$2.328 \text{ g/cm}^3$	$5.3267 \text{ g/cm}^3$	$5.32 \text{ g/cm}^3$
Atoms/ $\text{m}^3$	$5.0 \times 10^{28}$	$4.42 \times 10^{28}$	$4.42 \times 10^{28}$

# The thermodynamic properties of insulators depend on band edges

## Boltzmann approximation

The table below gives the contribution of electrons in intrinsic semiconductors and insulators to some thermodynamic quantities. These results were calculated in the Boltzmann approximation where it is assumed that the chemical potential lies in the band gap more than  $3k_B T$  from the band edge. The electronic contribution to the thermodynamic quantities are usually much smaller than the contribution of the phonons and thus the electronic components are often simply ignored.

	1-d	2-d
<b>Density of states</b> $m_e^*$ and $m_h^*$ are 'density of states' effective masses	$D(E) = \begin{cases} \frac{1}{\hbar\pi} \sqrt{\frac{2m_h^*}{(E_v - E)}} & E < E_v \\ 0 & E_v < E < E_c \\ \frac{1}{\hbar\pi} \sqrt{\frac{2m_e^*}{(E - E_c)}} & E > E_c \end{cases} \quad \text{J}^{-1} \text{m}^{-1}$	$D(E) = \begin{cases} \frac{m_h^*}{\hbar^2\pi} H(E_v - E) & E < E_v \\ 0 & E_v < E < E_c \\ \frac{m_e^*}{\hbar^2\pi} H(E - E_c) & E > E_c \end{cases} \quad \text{J}^{-1} \text{m}^{-2}$ <p><math>H(x) = 0</math> for <math>x &lt; 0</math> and <math>H(x) = 1</math> for <math>x &gt; 0</math></p>
<b>Density of states</b> $N_v$ and $N_c$ are the effective densities of states	$D(E) = \begin{cases} N_v(300) \sqrt{\frac{2}{300\pi k_B (E_v - E)}} & E < E_v \\ 0 & E_v < E < E_c \\ N_c(300) \sqrt{\frac{2}{300\pi k_B (E - E_c)}} & E > E_c \end{cases} \quad \text{J}^{-1} \text{m}^{-1}$	$D(E) = \begin{cases} \frac{N_v(300)}{300k_B} H(E_v - E) & E < E_v \\ 0 & E_v < E < E_c \\ \frac{N_c(300)}{300k_B} H(E - E_c) & E > E_c \end{cases} \quad \text{J}^{-1} \text{m}^{-2}$
<b>Density of electrons in the conduction band</b> $n = \int_{E_c}^{\infty} D(E) f(E) dE$	$n = \sqrt{\frac{m_e^* k_B T}{\hbar^2 \pi}} \exp\left(\frac{\mu - E_c}{k_B T}\right) \quad \text{m}^{-1}$ $= N_c \exp\left(\frac{\mu - E_c}{k_B T}\right)$	$n = \frac{m_e^* k_B T}{\hbar^2 \pi} \exp\left(\frac{\mu - E_c}{k_B T}\right) \quad \text{m}^{-2}$ $= N_c \exp\left(\frac{\mu - E_c}{k_B T}\right)$
<b>Density of holes in the valence band</b> $p = \int_{-\infty}^{E_v} D(E) (1 - f(E)) dE$	$p = \sqrt{\frac{m_h^* k_B T}{\hbar^2 \pi}} \exp\left(\frac{E_v - \mu}{k_B T}\right) \quad \text{m}^{-1}$ $= N_v \exp\left(\frac{\mu - E_c}{k_B T}\right)$	$p = \frac{m_h^* k_B T}{\hbar^2 \pi} \exp\left(\frac{E_v - \mu}{k_B T}\right) \quad \text{m}^{-2}$ $= N_v \exp\left(\frac{\mu - E_c}{k_B T}\right)$

# Law of mass action

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$$np = N_c \exp\left(\frac{\mu - E_c}{k_B T}\right) N_v \exp\left(\frac{E_v - \mu}{k_B T}\right)$$

$$np = N_c N_v \exp\left(\frac{-E_g}{k_B T}\right)$$

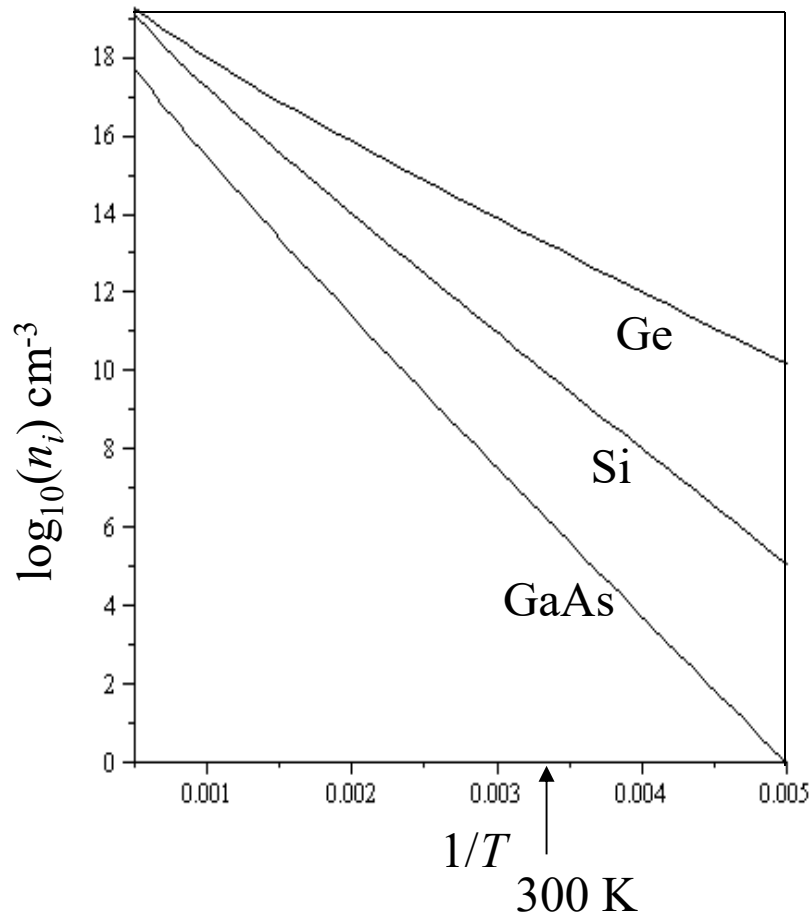
For intrinsic semiconductors (no impurities)

$$n = p = n_i = \sqrt{N_c N_v} \exp\left(\frac{-E_g}{2k_B T}\right)$$

For insulators,  $n_i \approx 0$ .

# Intrinsic carrier concentration $n_i$

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$$n_i = \sqrt{N_v N_c} \exp\left(-\frac{E_g}{2k_B T}\right)$$

# Chemical potential of an intrinsic semiconductor or an insulator

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$$n = p = N_c \exp\left(\frac{\mu - E_c}{k_B T}\right) = N_v \exp\left(\frac{E_v - \mu}{k_B T}\right)$$

$$\frac{N_v}{N_c} = \exp\left(\frac{\mu - E_c - E_v + \mu}{k_B T}\right)$$

$$\frac{2\mu}{k_B T} = \frac{E_c + E_v}{k_B T} + \ln\left(\frac{N_v}{N_c}\right)$$

$$\mu = \frac{E_c + E_v}{2} + \frac{k_B T}{2} \ln\left(\frac{N_v}{N_c}\right)$$

## Intrinsic semiconductors

In the Boltzmann approximation, the density of states of a semiconductor is,

$$D(E) = \begin{cases} \frac{(2m_h^*)^{3/2}}{2\pi^2 \hbar^3} \sqrt{E_v - E}, & \text{for } E < E_v \\ 0, & \text{for } E_v < E < E_c \\ \frac{(2m_e^*)^{3/2}}{2\pi^2 \hbar^3} \sqrt{E - E_c}, & \text{for } E_c < E \end{cases}$$

Here  $m_e^*$  and  $m_h^*$  are the 'density of states effective masses' for electrons and holes. Usually in the literature, effective density of states at 300 K is given instead of the 'density of states effective masses'. The relationship between the two is,

$$m_h^* = \frac{\pi \hbar^2}{300k_B} \left( \sqrt{2} N_v(300) \right)^{2/3}$$

$$m_e^* = \frac{\pi \hbar^2}{300k_B} \left( \sqrt{2} N_c(300) \right)^{2/3}$$

The density of states can therefore also be written as,

$$D(E) = \begin{cases} \frac{2N_v(300)}{\sqrt{\pi}} \left( \frac{1}{300k_B} \right)^{3/2} \sqrt{E_v - E}, & \text{for } E < E_v \\ 0, & \text{for } E_v < E < E_c \\ \frac{2N_c(300)}{\sqrt{\pi}} \left( \frac{1}{300k_B} \right)^{3/2} \sqrt{E - E_c}, & \text{for } E_c < E \end{cases}$$

In an intrinsic semiconductor, the density of electrons equals the density of holes. The intrinsic carrier concentration,  $n_i$ , depends exponentially on the bandgap,  $E_g$ . For most semiconductors the bandgap is a function of temperature. The plots on this page use the temperature dependence specified in the form below.

$$n = p = n_i = \sqrt{N_c \left( \frac{T}{300} \right)^{3/2} N_v \left( \frac{T}{300} \right)^{3/2} \exp\left(\frac{-E_g}{2k_B T}\right)}.$$

By setting the concentration of electrons equal to the concentration of holes, it is possible to solve for the chemical potential.

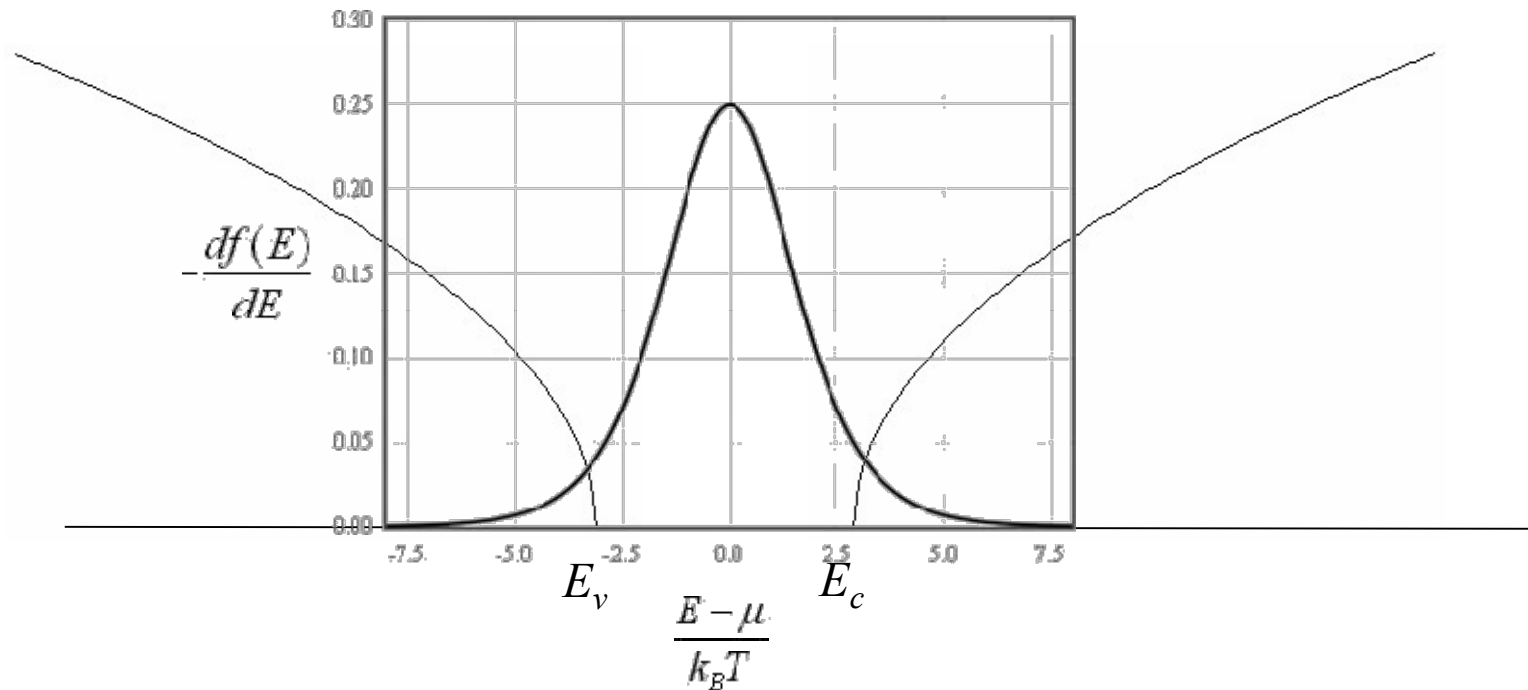
$$n = N_c(300) \left( \frac{T}{300} \right)^{3/2} \exp\left(\frac{\mu - E_c}{k_B T}\right) = p = N_v(300) \left( \frac{T}{300} \right)^{3/2} \exp\left(\frac{E_v - \mu}{k_B T}\right).$$

$$\mu = \frac{E_v + E_c}{2} + k_B T \ln\left(\frac{N_v(300)}{N_c(300)}\right).$$



# Narrow bandgap semiconductors

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Use the programs for metals for small bandgap semiconductors.

# Charged particle in a magnetic field

$$\vec{F} = -e\vec{v} \times \vec{B}$$

$$evB_z = \frac{mv^2}{R}$$

$$v = \omega_c R$$

$$\omega_c = \frac{eB_z}{m}$$



Magnetron

