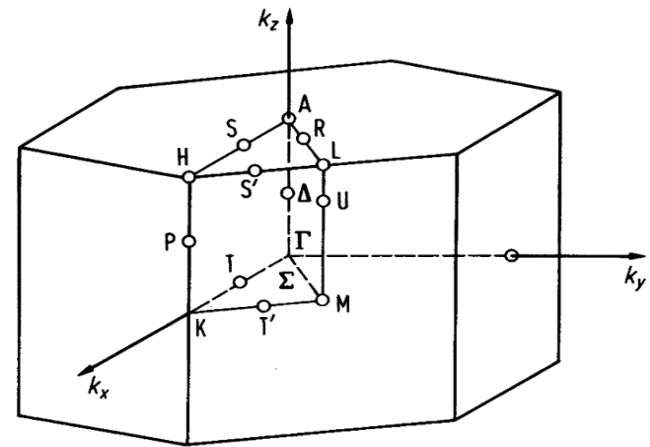
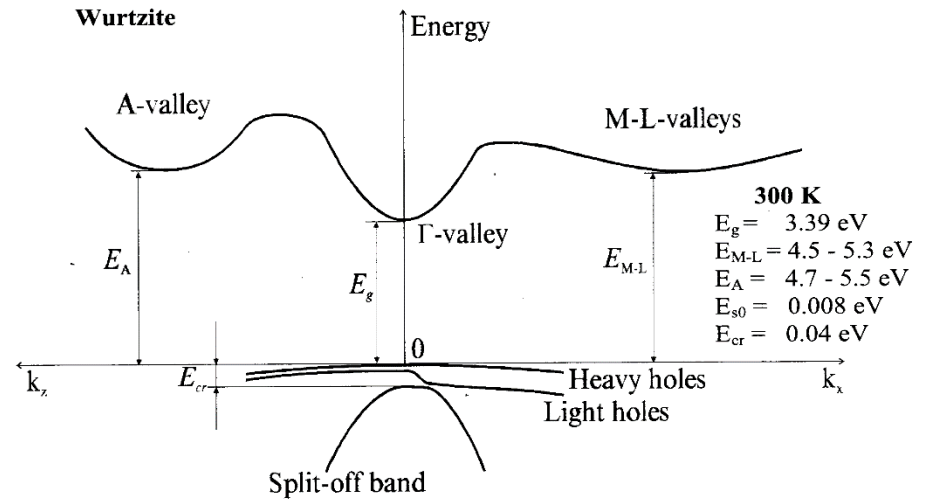
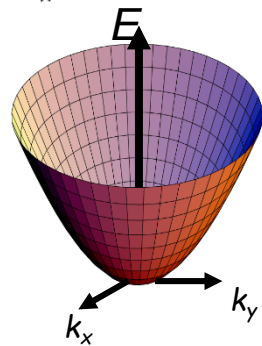
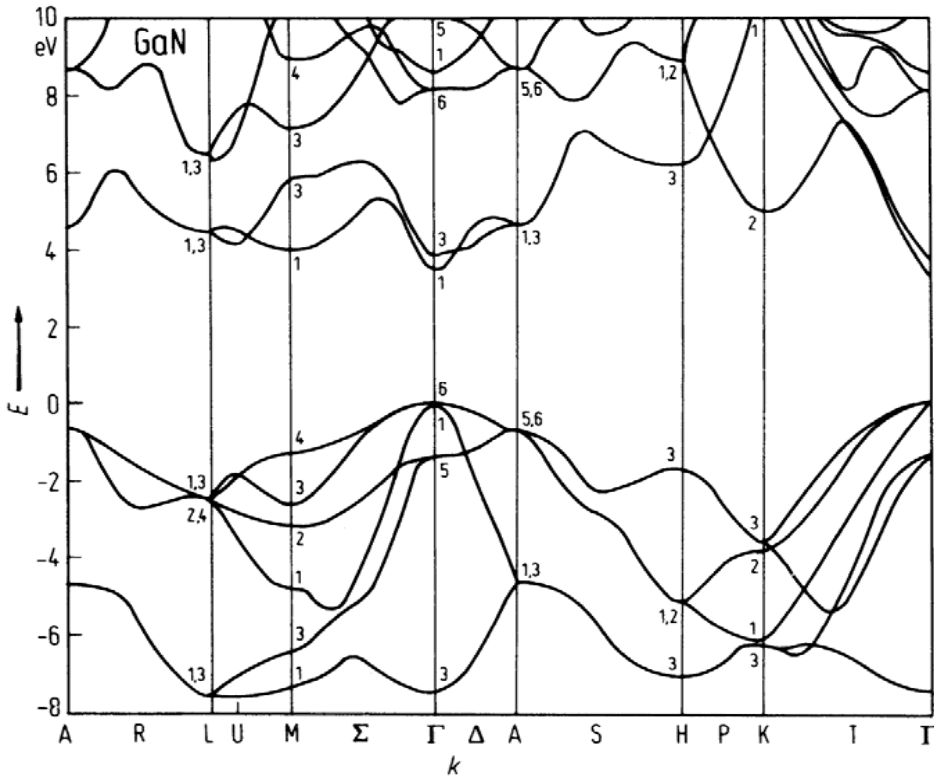


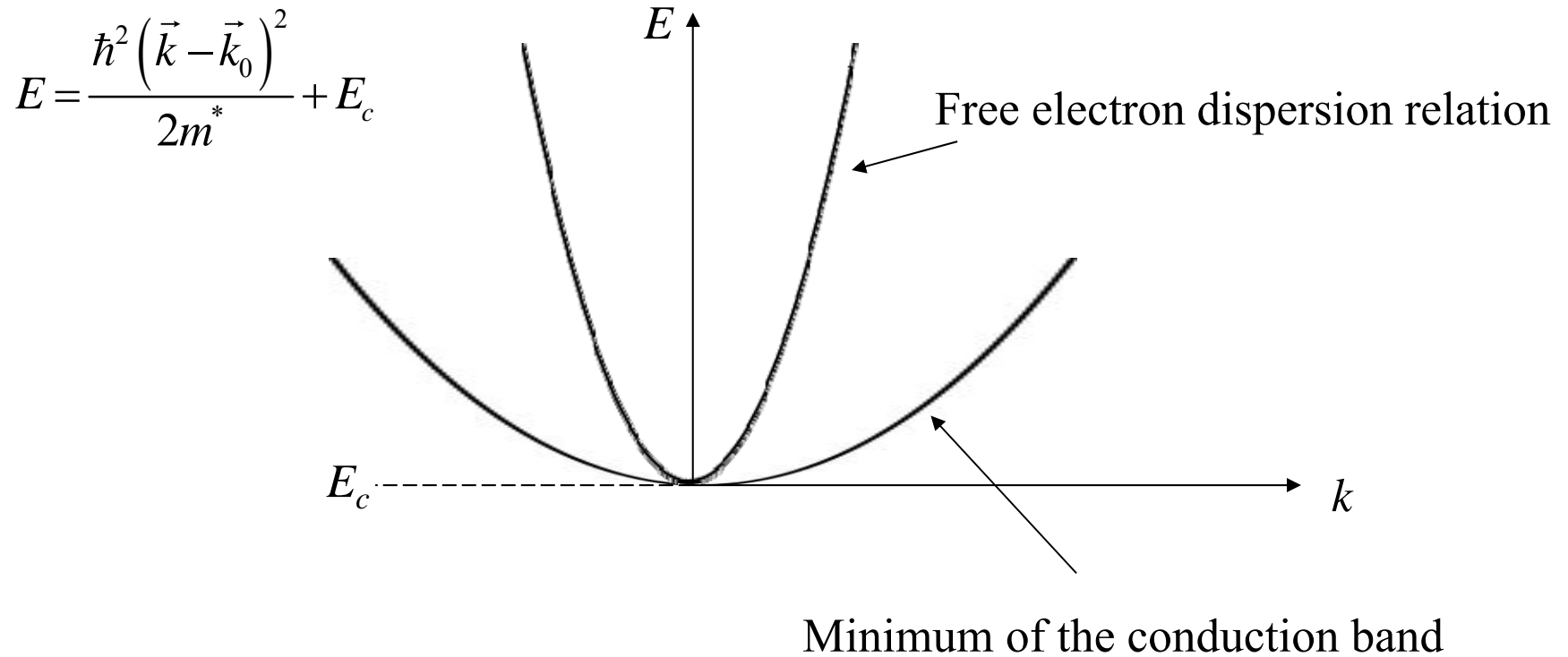
Semiconductors

GaN



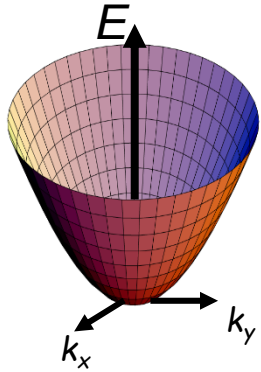
1st Brillouin zone of hcp

Conduction band minimum



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

Effective mass



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

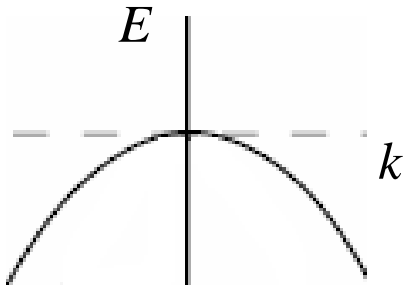
The parabola at the bottom of the conduction band does not have the same curvature as the free-electron dispersion relation. We define an effective mass to characterize the conduction band minimum.

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

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.



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

Charge carriers in the valence band are positively charged holes.

m_h^* = effective mass of holes

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

Holes

A completely filled band does not contribute to the current.

$$\begin{aligned}\vec{j} &= \int_{\text{filled states}} -e\vec{v}(\vec{k})D(\vec{k})f(\vec{k})d\vec{k} \\ &= \int_{\text{band}} -e\vec{v}(\vec{k})D(\vec{k})f(\vec{k})d\vec{k} - \int_{\text{empty states}} -e\vec{v}(\vec{k})D(\vec{k})f(\vec{k})d\vec{k} \\ &= \int_{\text{empty states}} e\vec{v}(\vec{k})D(\vec{k})f(\vec{k})d\vec{k}\end{aligned}$$

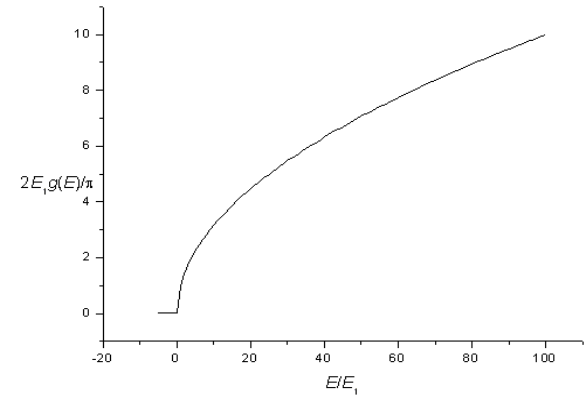
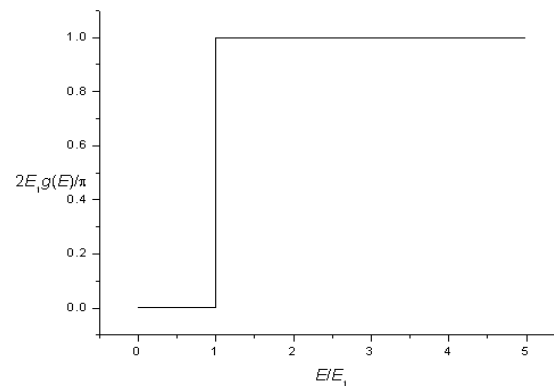
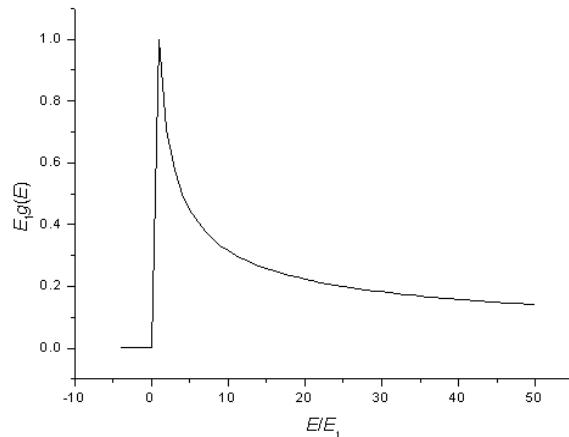
Holes have a positive charge and a positive mass.

Free electron Fermi gas

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

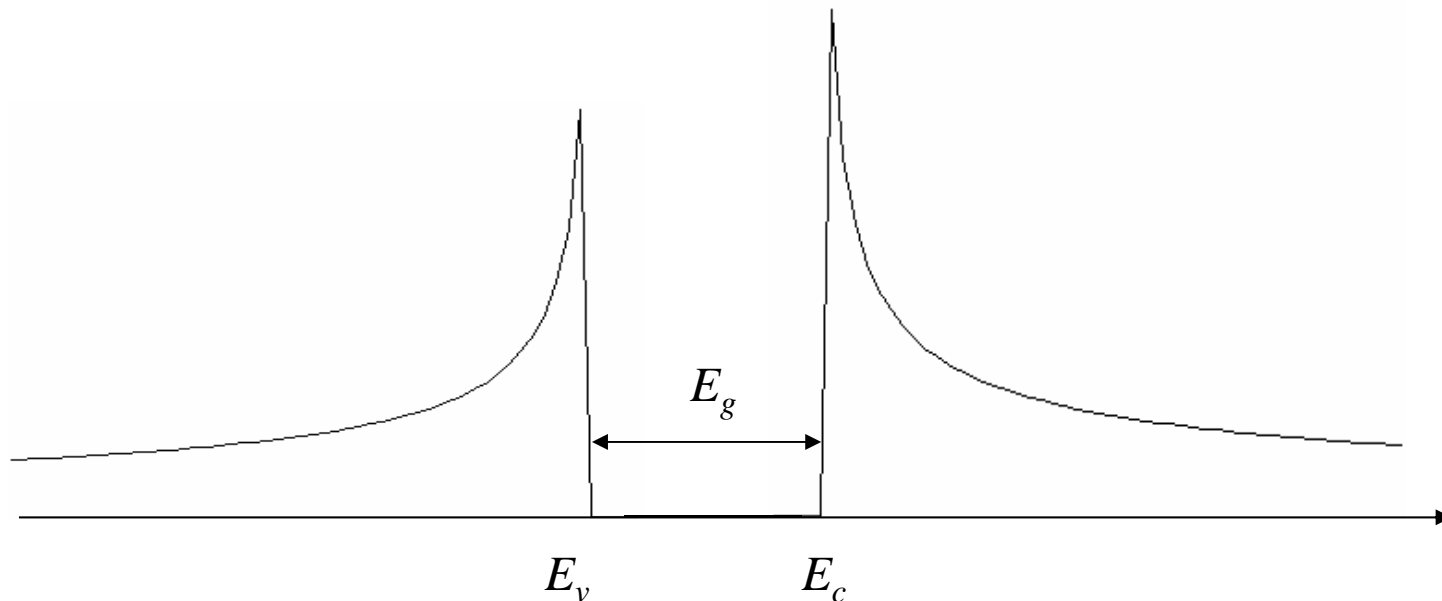
$$2 - d \quad D(E) = \frac{m}{\hbar^2 \pi} = \frac{n}{E_F} \quad \text{J}^{-1} \text{m}^{-2}$$

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



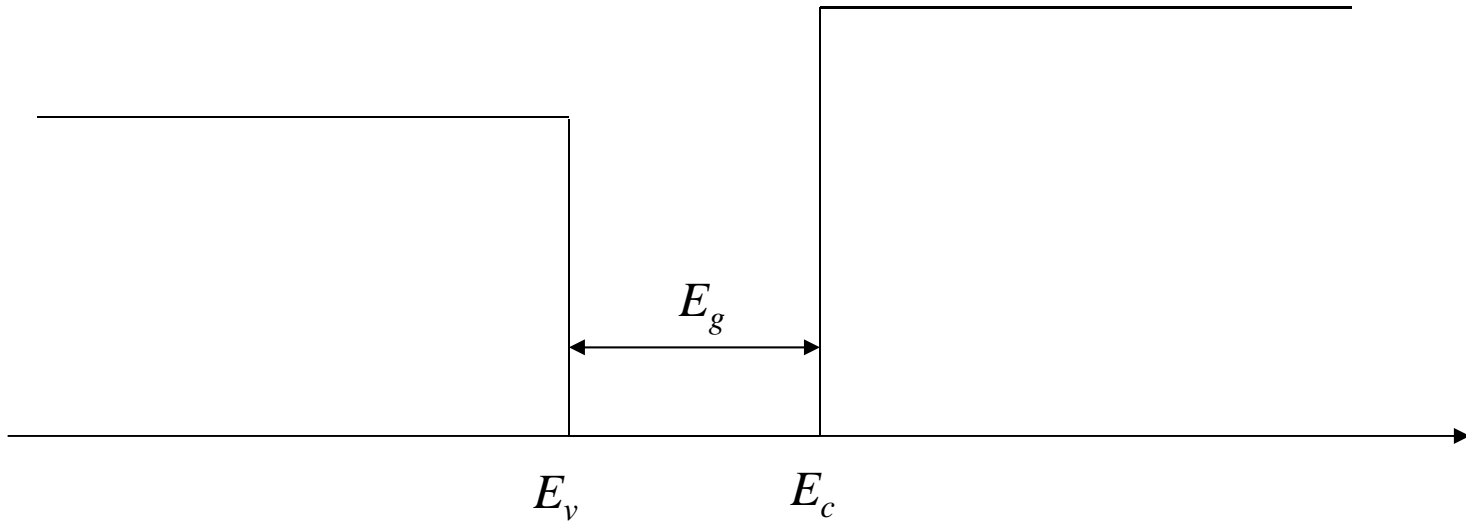
Semiconductors and insulators - 1d

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



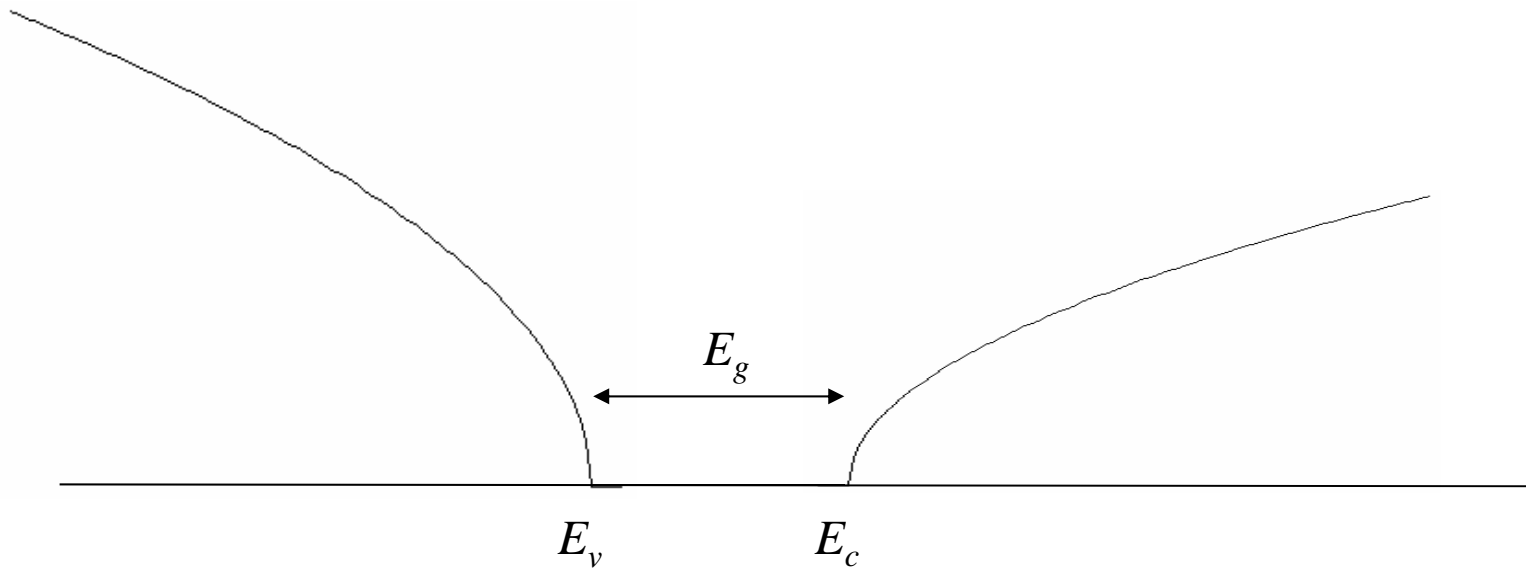
Semiconductors and insulators - 2d

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



Semiconductors and insulators - 3d

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



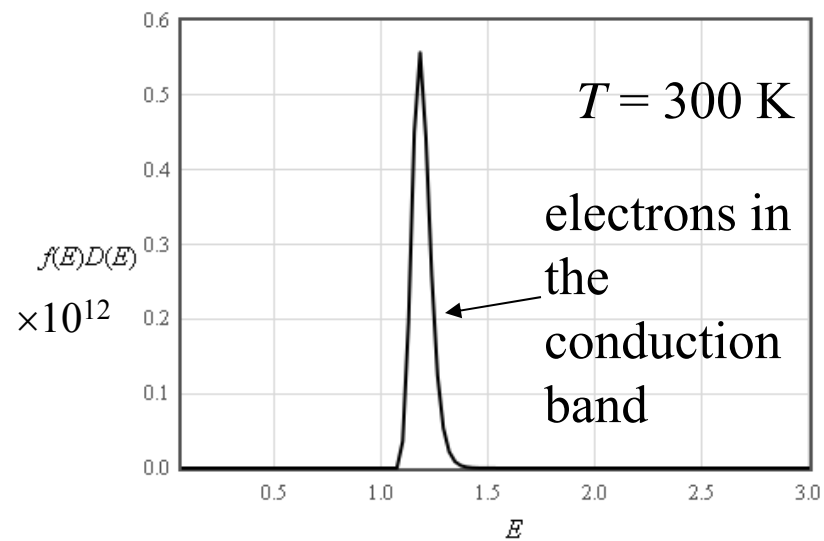
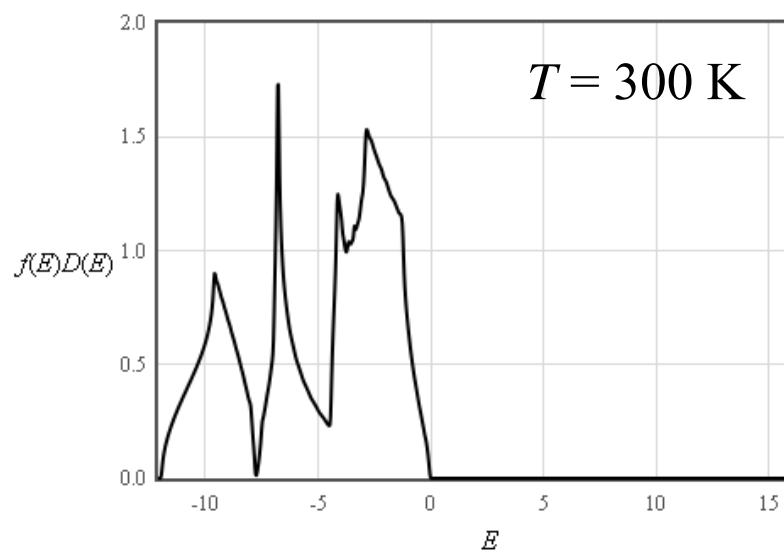
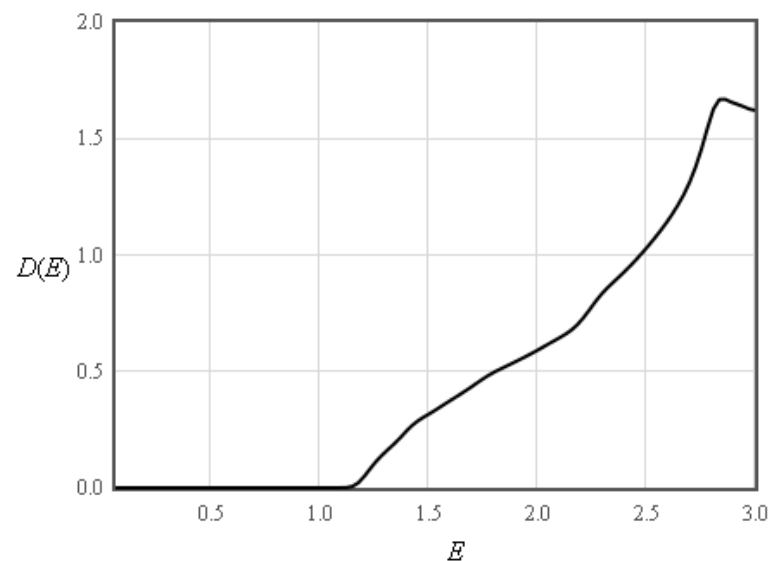
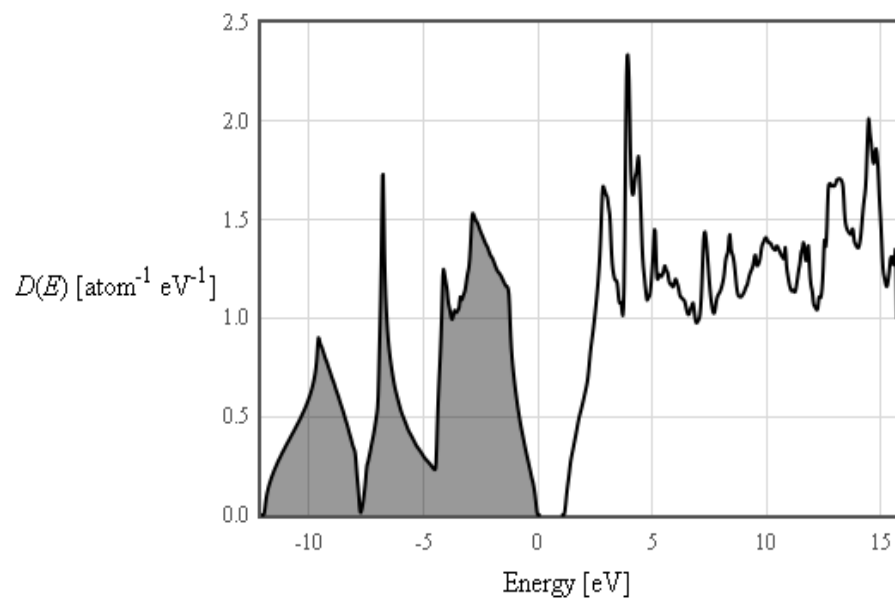
The electrical contribution to the thermodynamic properties of insulators depend on band edges

Boltzmann approximation

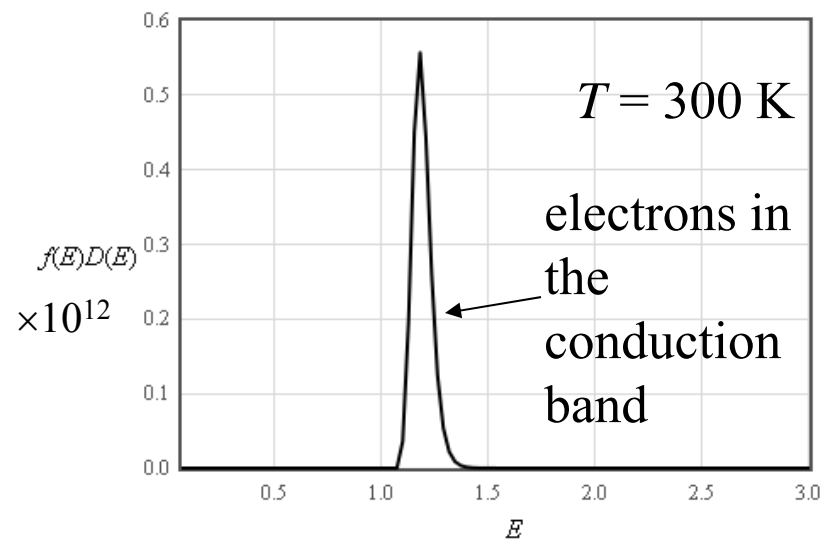
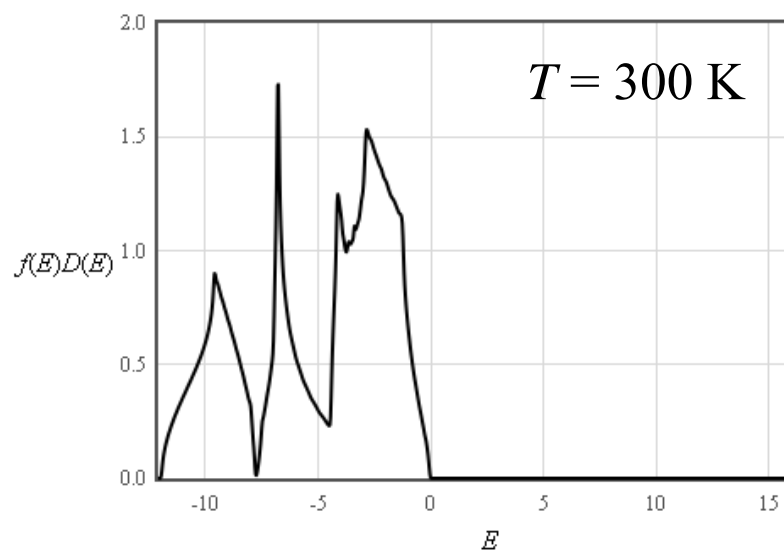
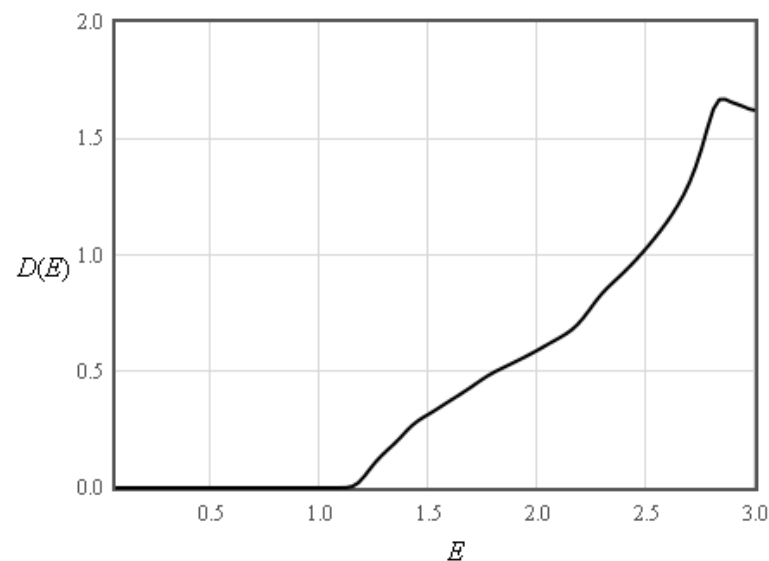
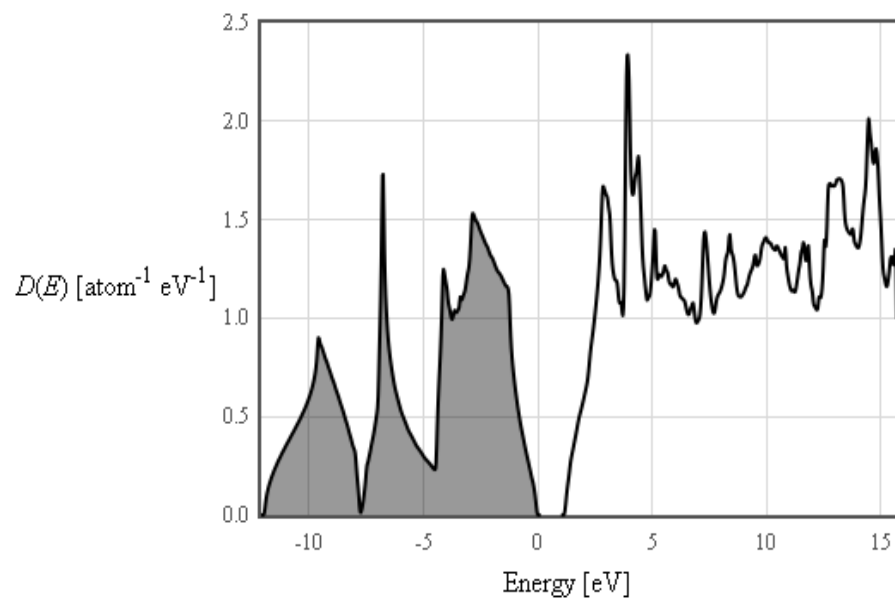
The table below gives the contribution of electrons in intrinsic semiconductors and insulators to some thermodynamic quantities. These results were calculated in the Boltzmann approximation where it is assumed that the chemical potential lies in the band gap more than $3k_B T$ from the band edge. The 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
Density of states m_e^* and m_h^* are 'density of states' effective masses	$D(E) = \begin{cases} \frac{1}{\hbar\pi} \sqrt{\frac{2m_h^*}{(E_v - E)}} & E < E_v \\ 0 & E_v < E < E_c \\ \frac{1}{\hbar\pi} \sqrt{\frac{2m_e^*}{(E - E_c)}} & E > E_c \end{cases} \quad \text{J}^{-1} \text{m}^{-1}$	$D(E) = \begin{cases} \frac{m_h^*}{\hbar^2\pi} H(E_v - E) & E < E_v \\ 0 & E_v < E < E_c \\ \frac{m_e^*}{\hbar^2\pi} H(E - E_c) & E > E_c \end{cases} \quad \text{J}^{-1} \text{m}^{-2}$ $H(x) = 0 \text{ for } x < 0 \text{ and } H(x) = 1 \text{ for } x > 0$
Density of states N_v and N_c are the effective densities of states	$D(E) = \begin{cases} N_v(300) \sqrt{\frac{2}{300\pi k_B (E_v - E)}} & E < E_v \\ 0 & E_v < E < E_c \\ N_c(300) \sqrt{\frac{2}{300\pi k_B (E - E_c)}} & E > E_c \end{cases} \quad \text{J}^{-1} \text{m}^{-1}$	$D(E) = \begin{cases} \frac{N_v(300)}{300k_B} H(E_v - E) & E < E_v \\ 0 & E_v < E < E_c \\ \frac{N_c(300)}{300k_B} H(E - E_c) & E > E_c \end{cases} \quad \text{J}^{-1} \text{m}^{-2}$
Density of electrons in the conduction band $n = \int_{E_c}^{\infty} D(E) f(E) dE$	$n = \sqrt{\frac{m_e^* k_B T}{\hbar^2 \pi}} \exp\left(\frac{\mu - E_c}{k_B T}\right) \quad \text{m}^{-1}$ $= N_c \exp\left(\frac{\mu - E_c}{k_B T}\right)$	$n = \frac{m_e^* k_B T}{\hbar^2 \pi} \exp\left(\frac{\mu - E_c}{k_B T}\right) \quad \text{m}^{-2}$ $= N_c \exp\left(\frac{\mu - E_c}{k_B T}\right)$
Density of holes in the valence band $p = \int_{-\infty}^{E_v} D(E) (1 - f(E)) dE$	$p = \sqrt{\frac{m_h^* k_B T}{\hbar^2 \pi}} \exp\left(\frac{E_v - \mu}{k_B T}\right) \quad \text{m}^{-1}$ $= N_v \exp\left(\frac{\mu - E_c}{k_B T}\right)$	$p = \frac{m_h^* k_B T}{\hbar^2 \pi} \exp\left(\frac{E_v - \mu}{k_B T}\right) \quad \text{m}^{-2}$ $= N_v \exp\left(\frac{\mu - E_c}{k_B T}\right)$

Silicon density of states



Silicon density of states



Silicon valence bands

$$E_{v,th} = -\frac{\hbar^2}{2m_e} \left(4.1k^2 - \sqrt{1.21k^4 + 4.1(k_x^2k_y^2 + k_x^2k_z^2 + k_y^2k_z^2)} \right),$$

$$E_{v,hh} = -\frac{\hbar^2}{2m_e} \left(4.1k^2 + \sqrt{1.21k^4 + 4.1(k_x^2k_y^2 + k_x^2k_z^2 + k_y^2k_z^2)} \right),$$

$$E_{v,so} = -E_{so} - \frac{\hbar^2k^2}{2m_{so}}.$$

