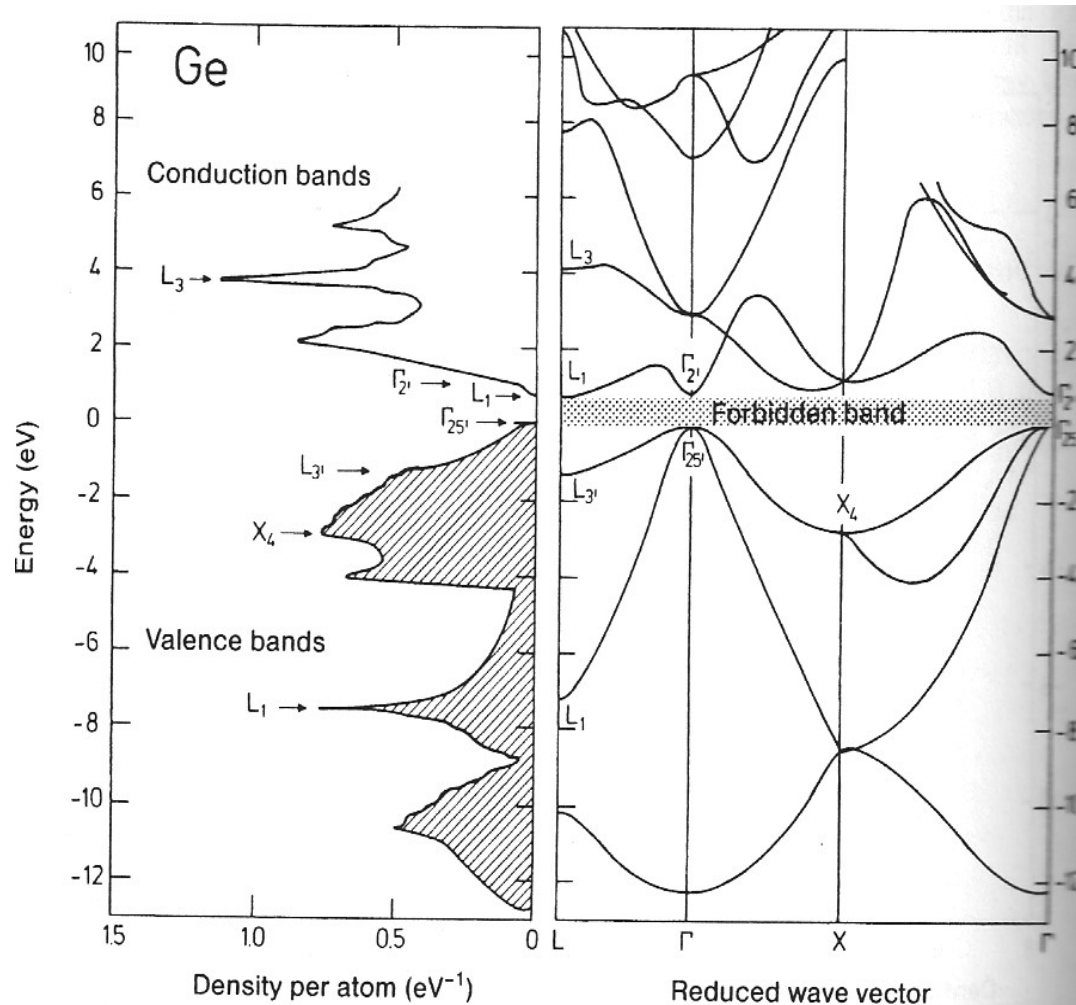


# Semiconductors

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# Semiconductors



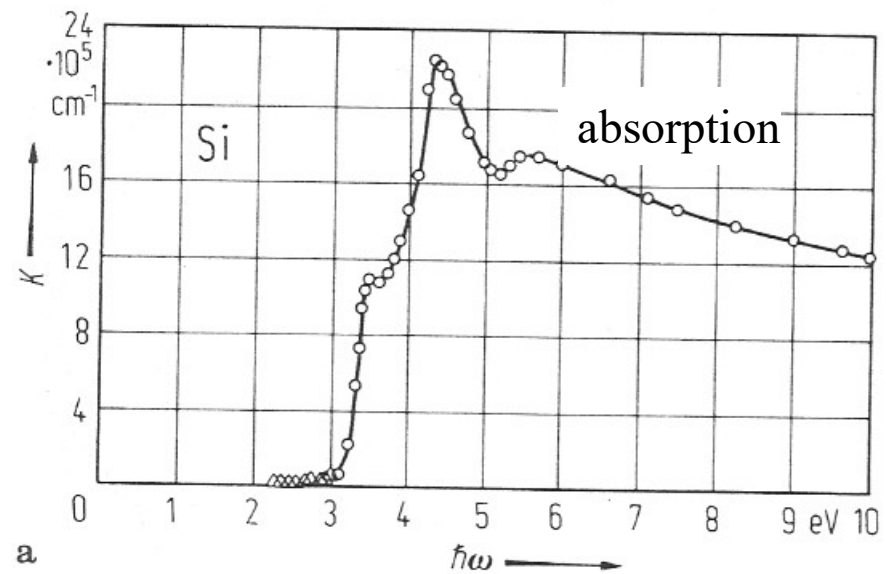
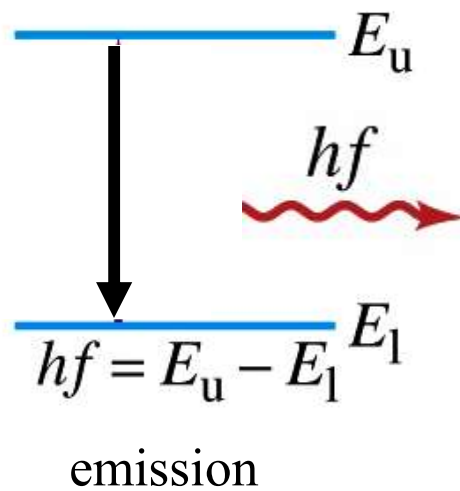
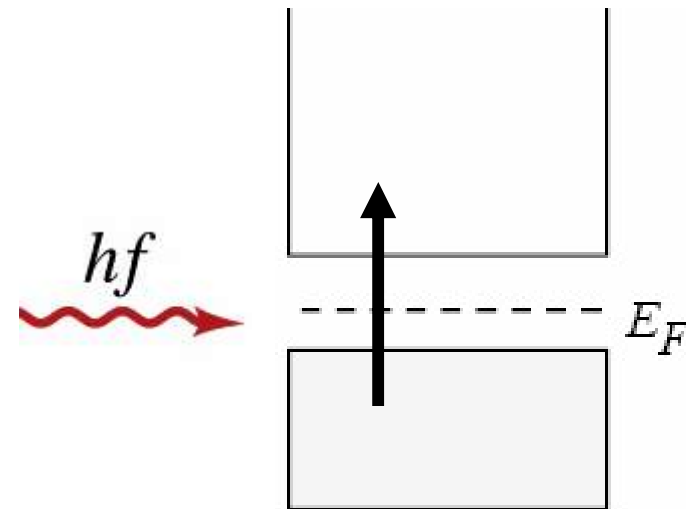
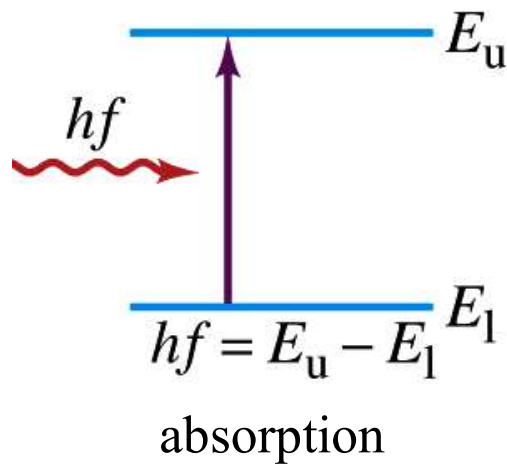
Conduction band

Valence band

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

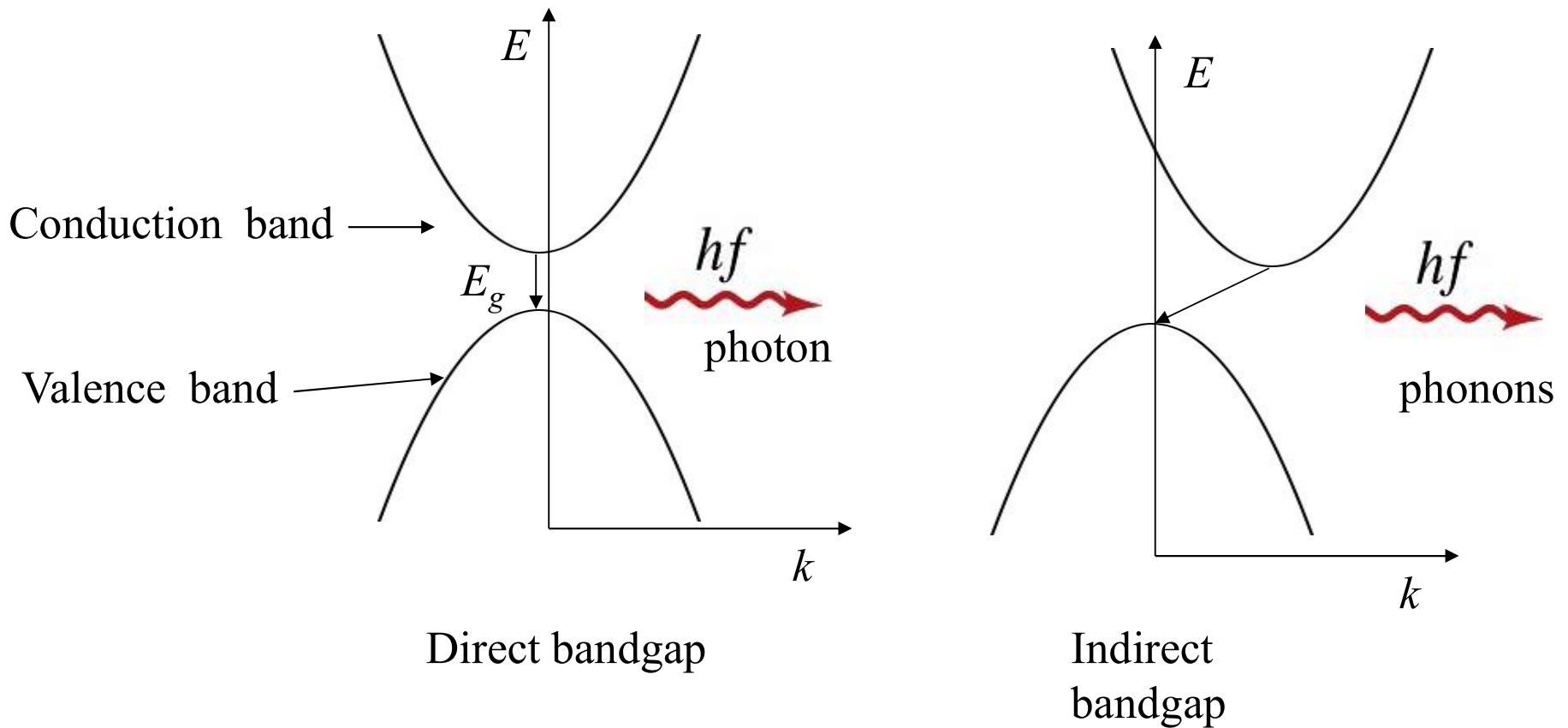
From Ibach & Lueth

# Absorption and emission of photons



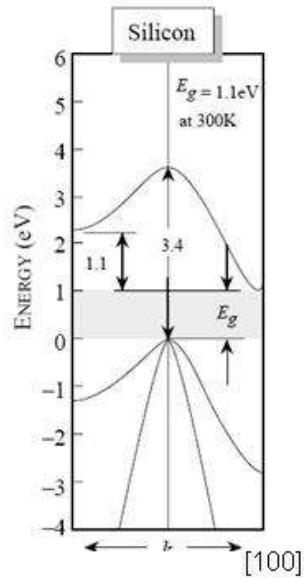
# Direct and indirect band gaps

---

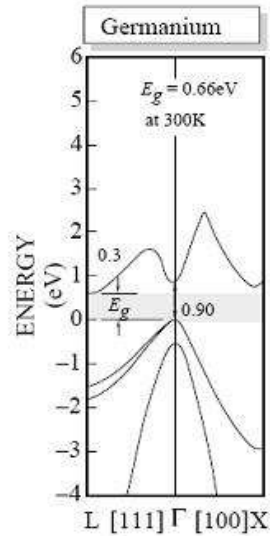


Direct bandgap semiconductors are used for optoelectronics

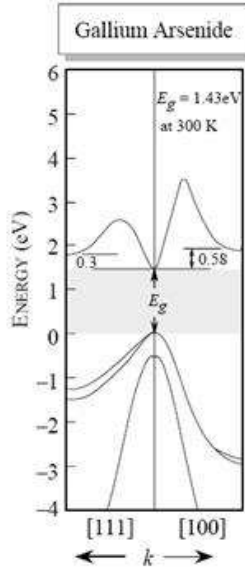
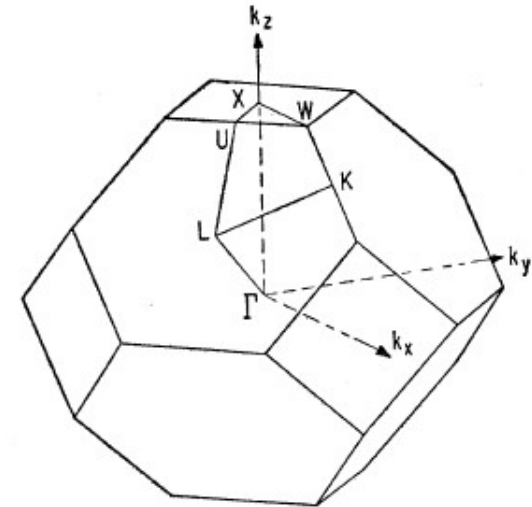
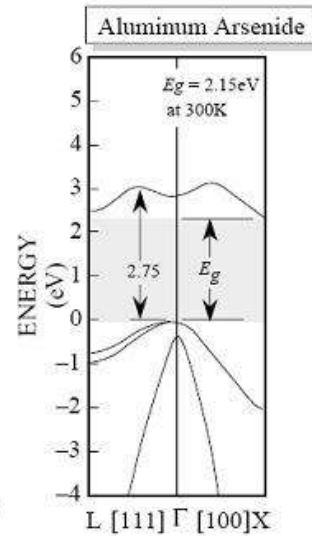
# Semiconductors



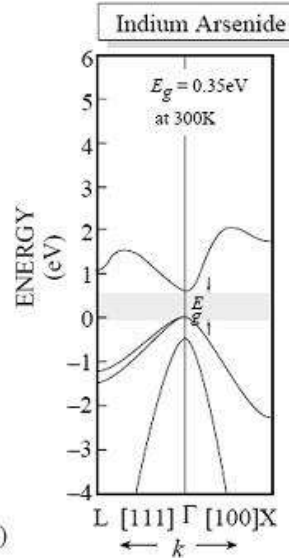
(a)



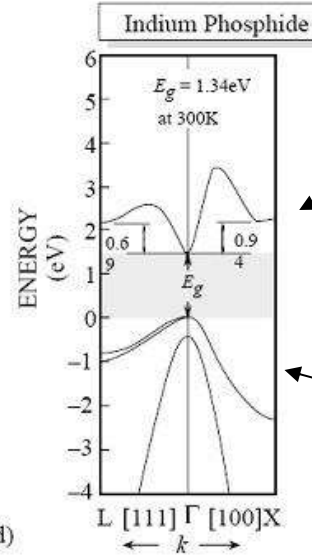
(b)



(c)



(d)



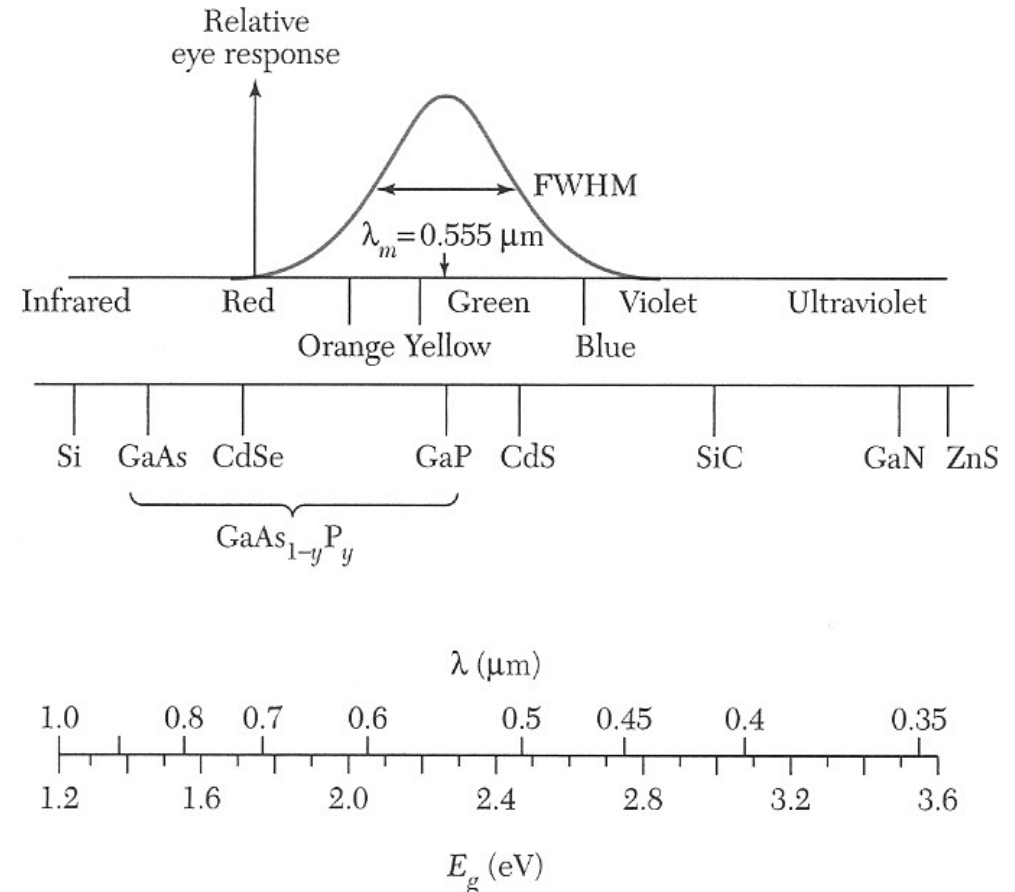
Conduction band

Valence band

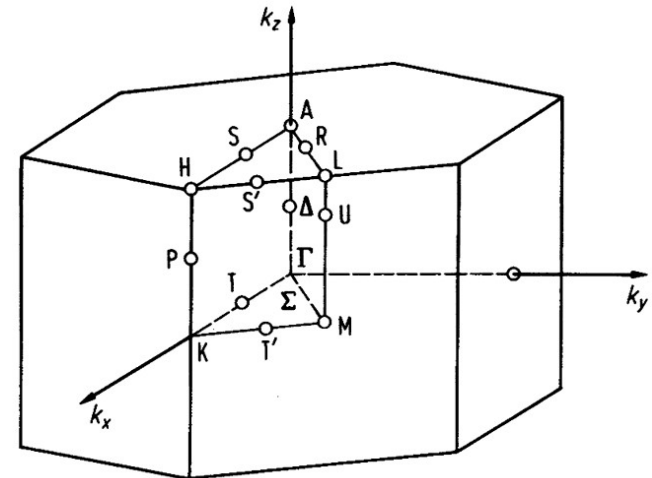
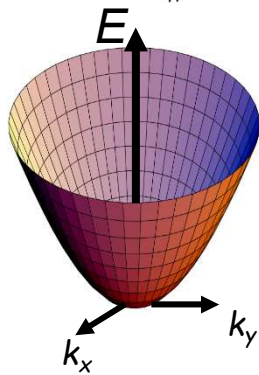
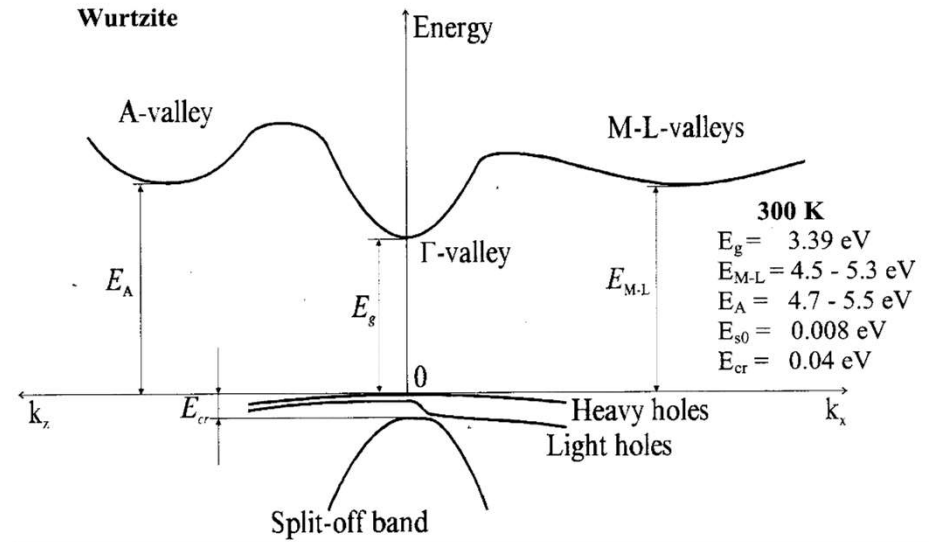
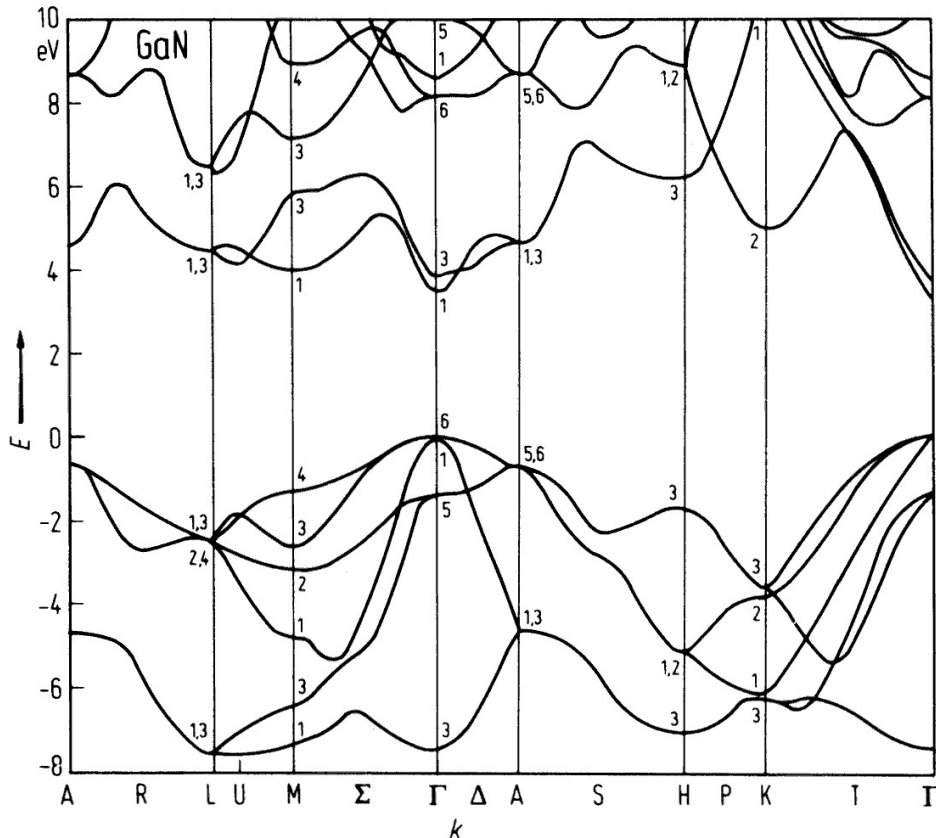
**TABLE 1 Common III-V materials used to produce LEDs and their emission wavelengths.**

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



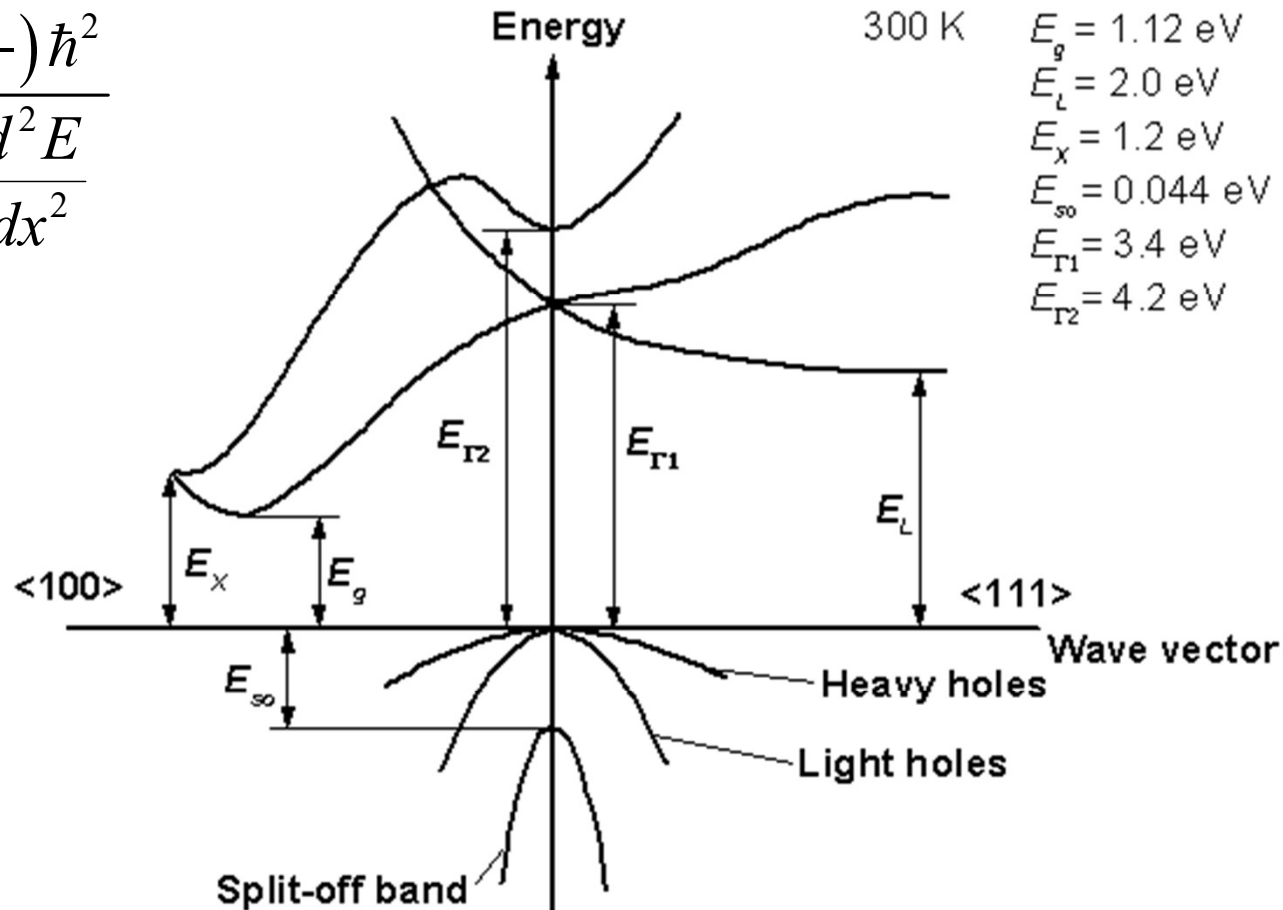
# GaN



1st Brillouin zone of hcp

# Silicon

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

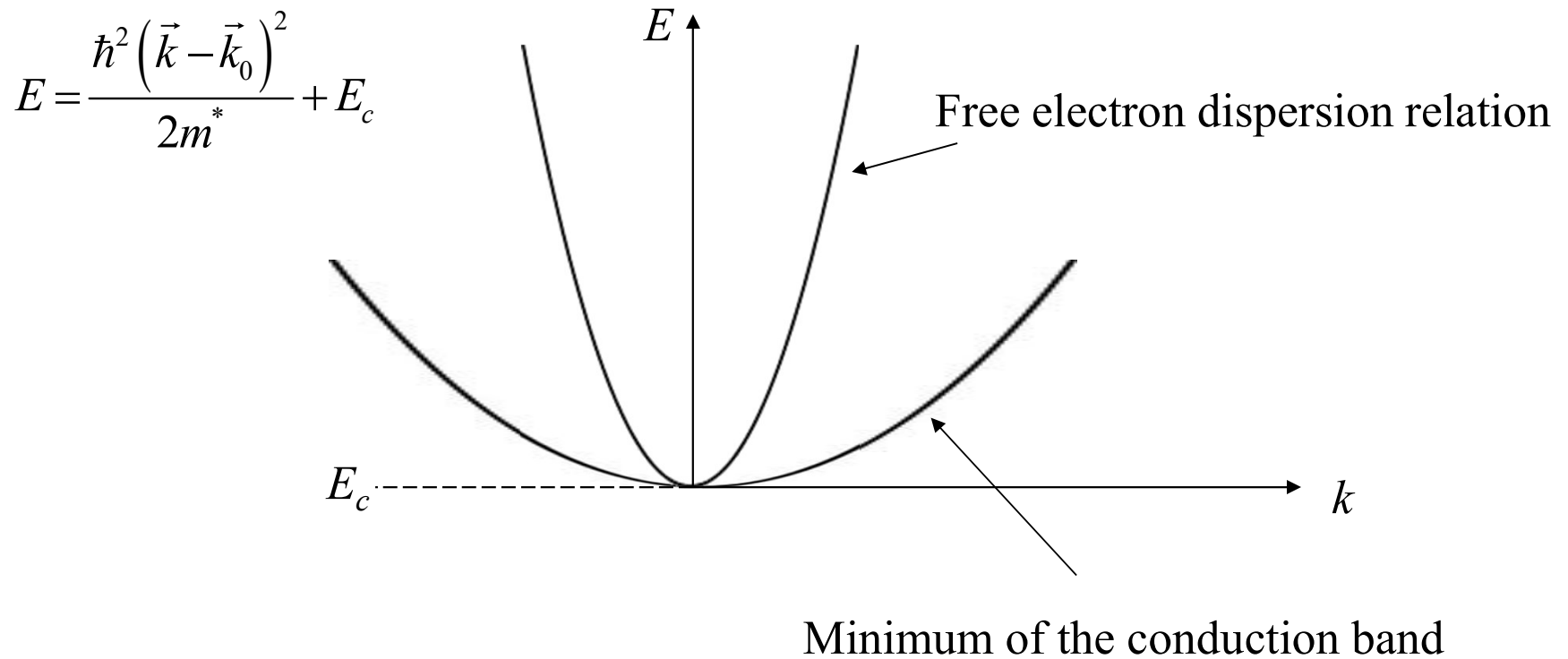


[http://www.matprop.ru/Si\\_bandstr#Basic](http://www.matprop.ru/Si_bandstr#Basic)



# Conduction band minimum

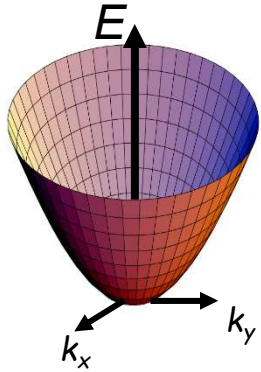
---



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.

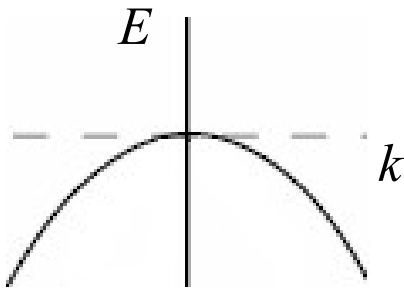
$$m^* = \frac{\hbar^2}{\frac{d^2 E(\vec{k})}{dk_x^2}}$$

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

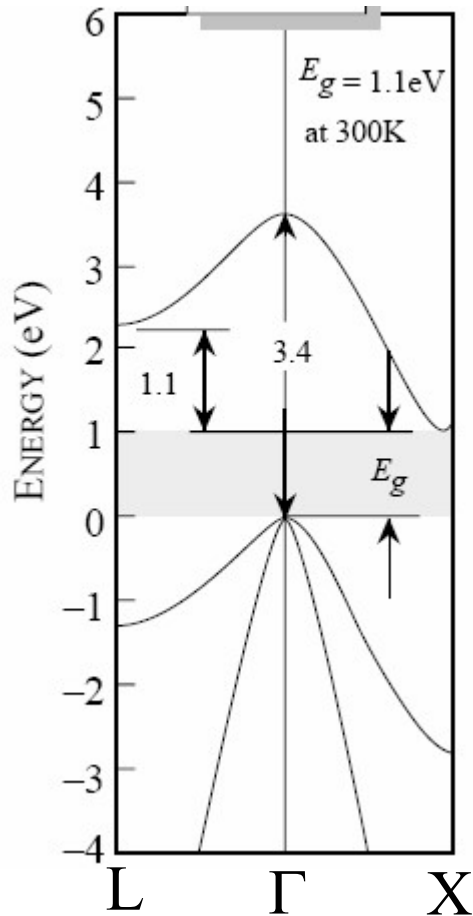
---

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.

# Effective Mass



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

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

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

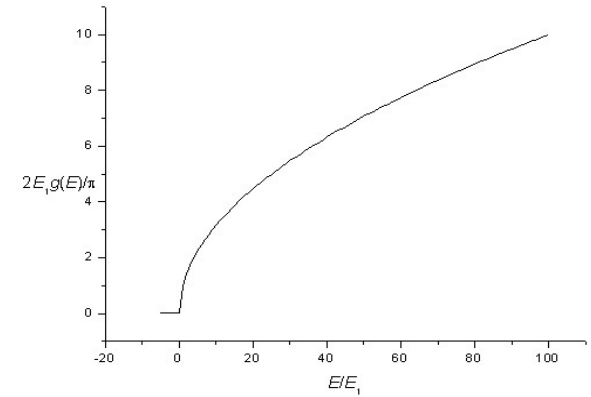
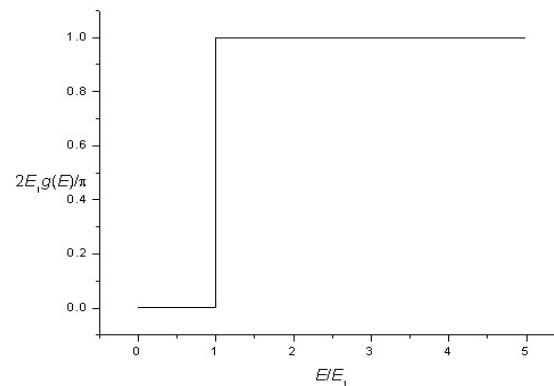
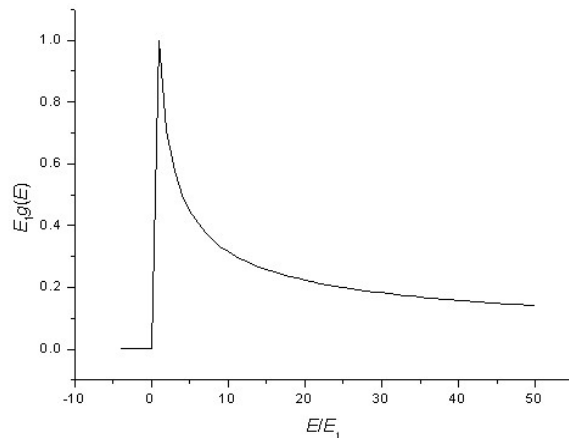
$$m_h^* = \frac{-\hbar^2}{\frac{d^2 E}{dk_x^2}}$$

# Free electron Fermi gas

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

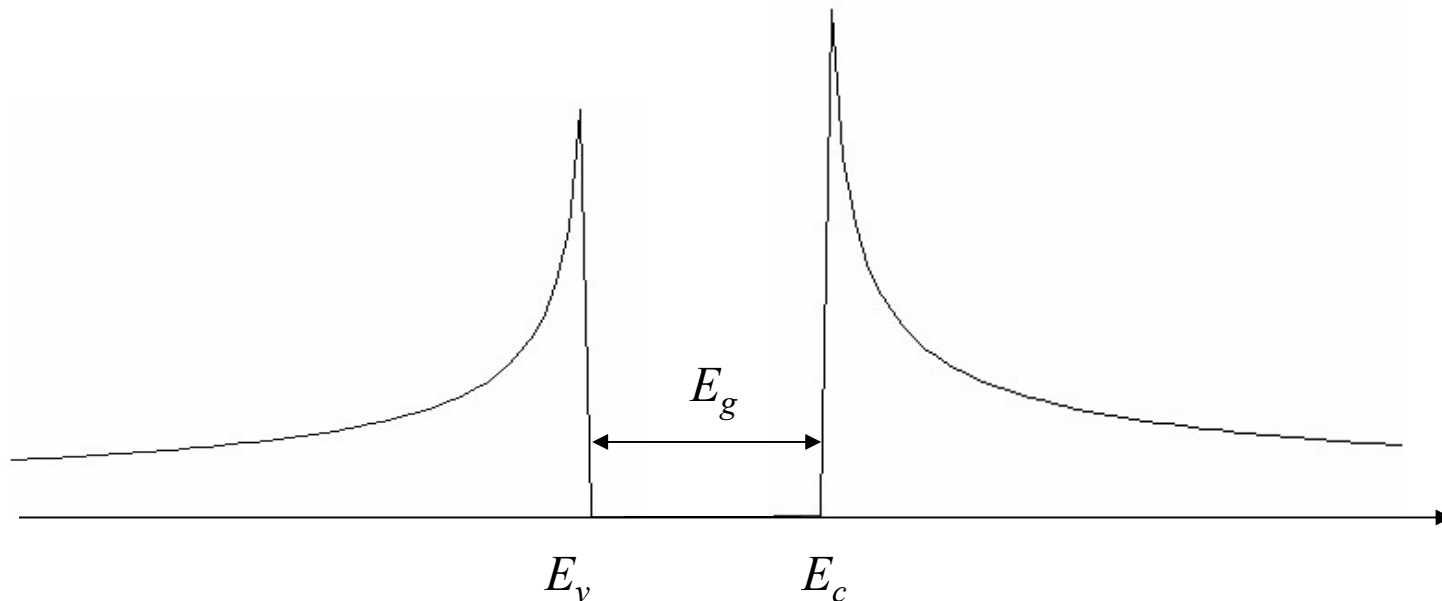
2 - d 
$$D(E) = \frac{m}{\hbar^2 \pi} = \frac{n}{E_F} \quad \text{J}^{-1} \text{m}^{-2}$$

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

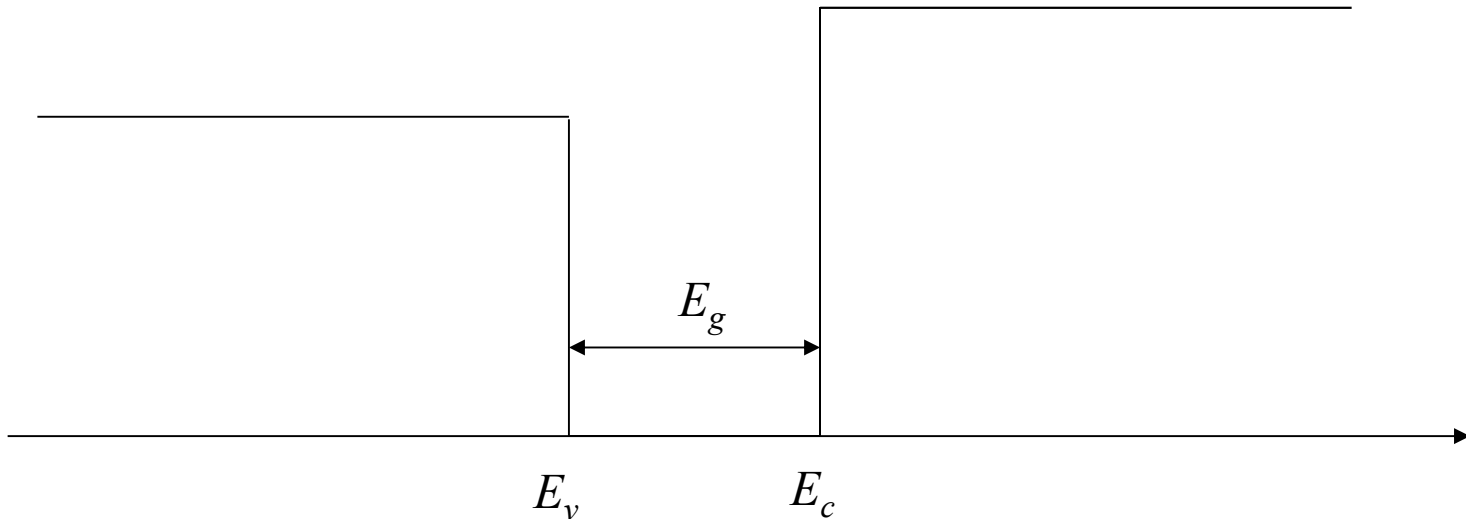
$$E = \frac{\hbar^2(\vec{k} - \vec{k}_0)^2}{2m^*}$$
$$D(E) = \begin{cases} \frac{D_c}{\sqrt{(E_v - E)}} & E < E_v \\ 0 & E_v < E < E_c \\ \frac{D_v}{\sqrt{(E - E_c)}} & E_c < E \end{cases} \quad \text{J}^{-1}\text{m}^{-3}$$



# Semiconductors and insulators - 2d

---

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

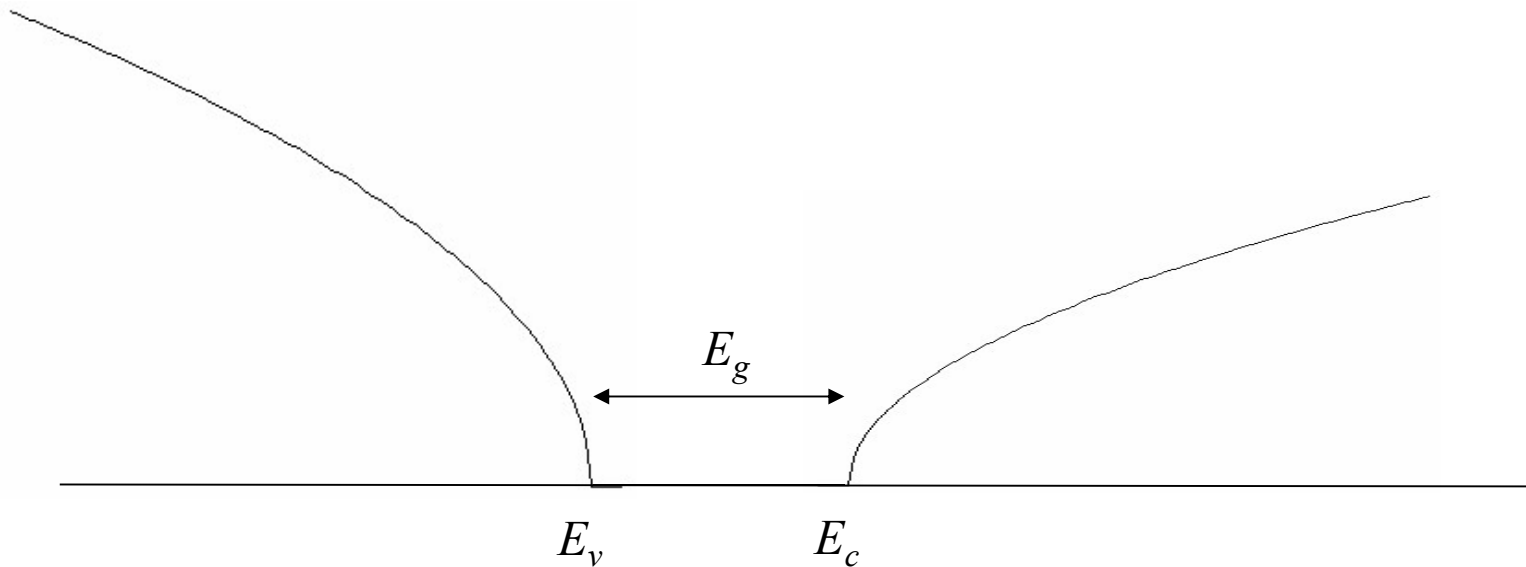




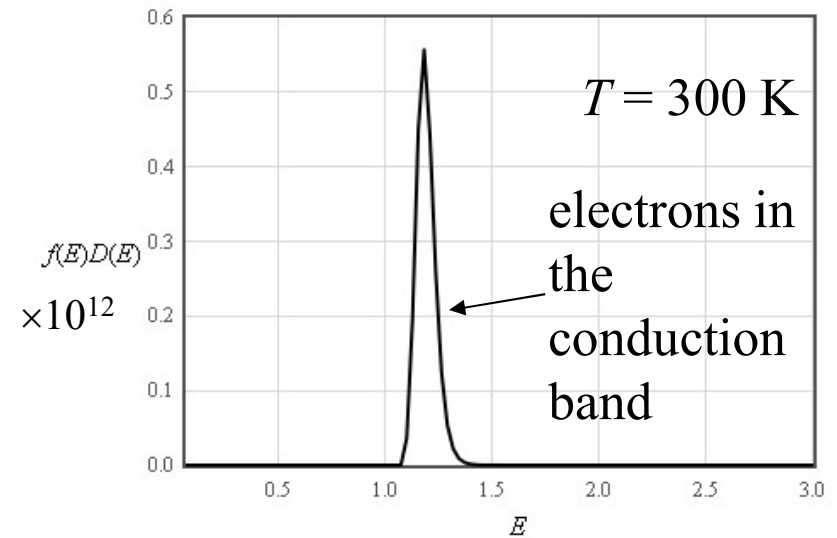
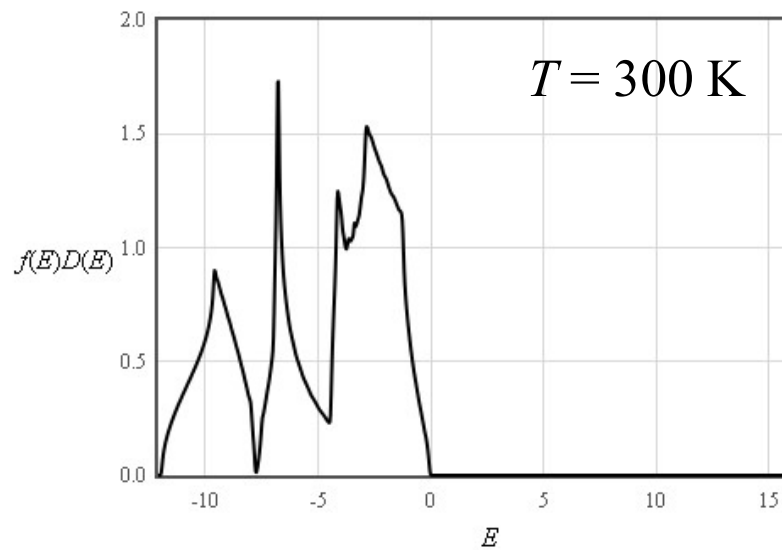
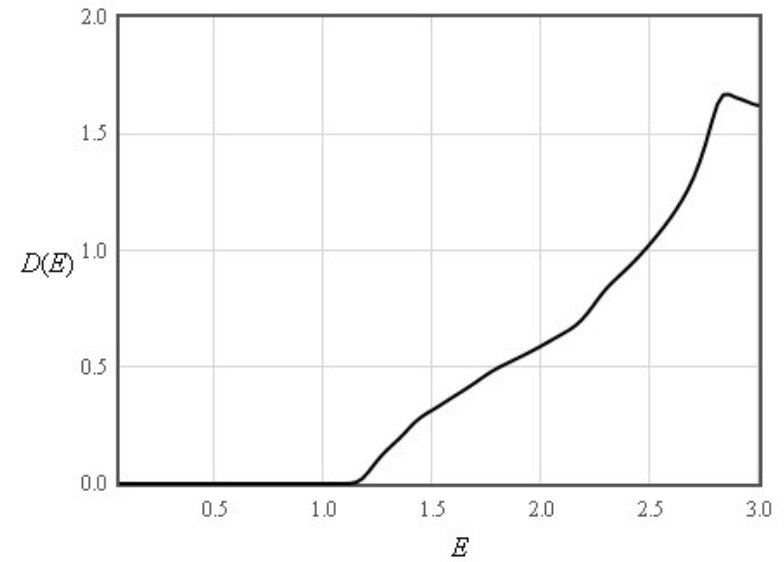
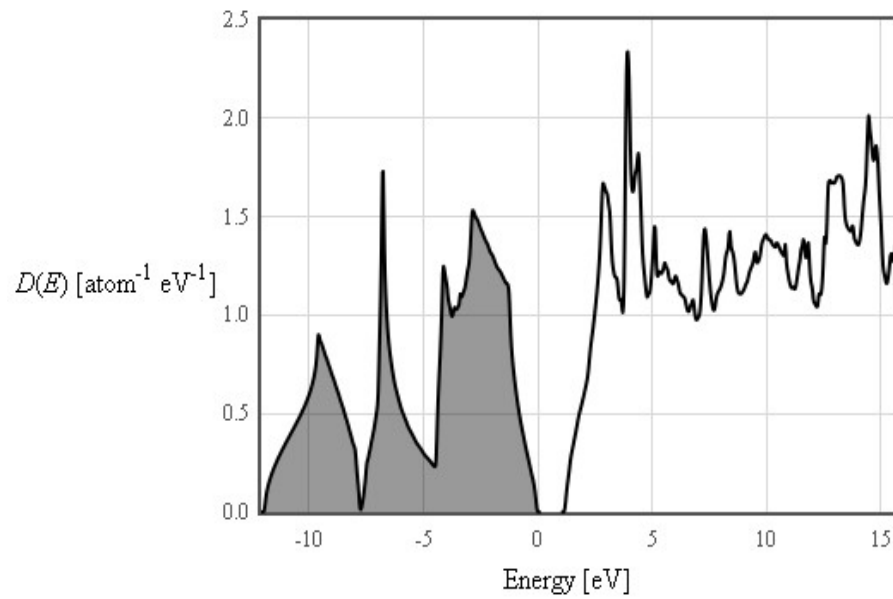
# Semiconductors and insulators - 3d

---

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



# Silicon density of states



# Boltzmann Approximation

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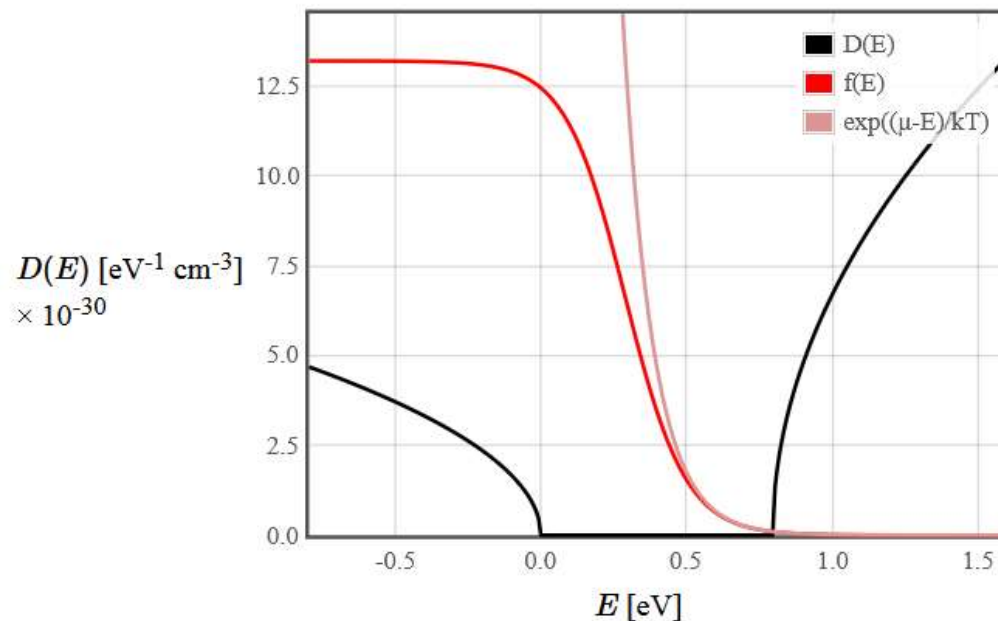
# Density of electrons in the conduction band

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

$$D(E) = D_c \sqrt{E - E_c}$$

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

Boltzmann approximation  
 $E_c - \mu > 3k_B T$



$$n = \int_{E_c}^{\infty} D(E) f(E) dE \approx D_c \int_{E_c}^{\infty} \exp\left(\frac{\mu - E}{k_B T}\right) \sqrt{E - E_c} dE$$

# Density of electrons in the conduction band

---

$$n = \int_{E_c}^{\infty} D(E) f(E) dE \approx D_c \int_{E_c}^{\infty} \exp\left(\frac{\mu - E}{k_B T}\right) \sqrt{E - E_c} dE$$
$$= D_c \exp\left(\frac{\mu - E_c}{k_B T}\right) \int_{E_c}^{\infty} \exp\left(-\frac{E - E_c}{k_B T}\right) \sqrt{E - E_c} dE$$

$$x = E - E_c \quad \int_0^{\infty} \sqrt{x} \exp\left(\frac{-x}{k_B T}\right) dx = \frac{2}{\sqrt{\pi}} (k_B T)^{3/2}$$

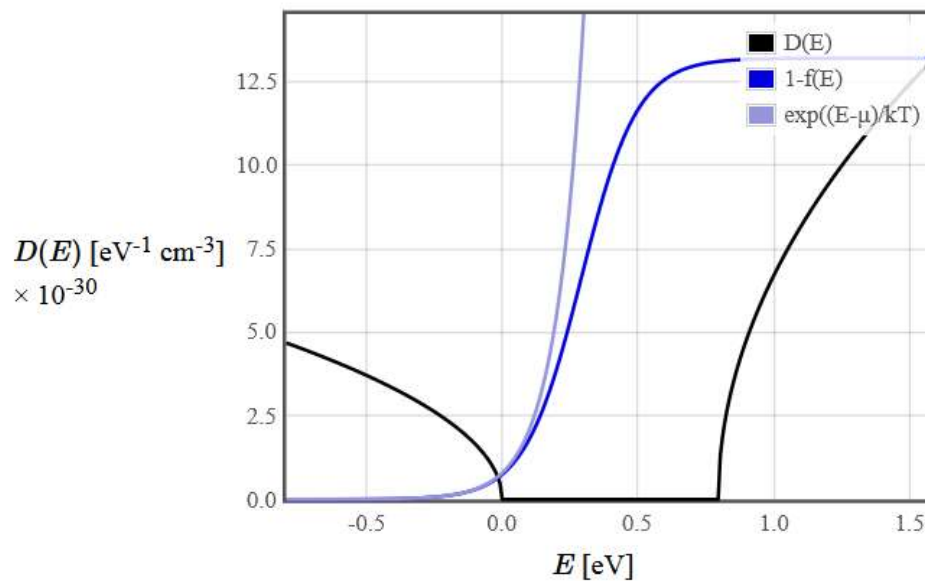
$$n = N_c(T) \exp\left(\frac{\mu - E_c}{k_B T}\right) = \frac{2D_c}{\sqrt{\pi}} (k_B T)^{3/2} \exp\left(\frac{\mu - E_c}{k_B T}\right)$$

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

# Density of holes in the valence band

$$D(E) = D_v \sqrt{E_v - E}$$

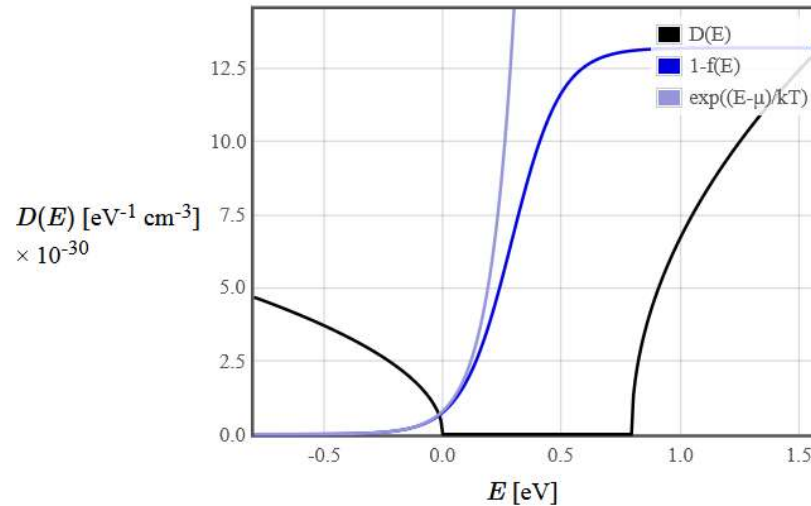
$$1 - f(E) = 1 - \frac{1}{1 + \exp\left(\frac{E - \mu}{k_B T}\right)} \approx \exp\left(\frac{E - \mu}{k_B T}\right)$$



Boltzmann  
approximation  
 $\mu - E_v > 3k_B T$

$$p = \int_{-\infty}^{E_v} D(E) (1 - f(E)) dE \approx D_v \int_{-\infty}^{E_v} \exp\left(\frac{E - \mu}{k_B T}\right) \sqrt{E_v - E} dE$$

# Density of holes in the valence band



$$p = \int_{-\infty}^{E_v} D(E)(1-f(E))dE \approx D_v \int_{-\infty}^{E_v} \exp\left(\frac{E-\mu}{k_B T}\right) \sqrt{E_v-E} dE$$

$$p = N_v \exp\left(\frac{E_v - \mu}{k_B T}\right) = \frac{2D_v}{\sqrt{\pi}} (k_B T)^{3/2} \exp\left(\frac{E_v - \mu}{k_B T}\right)$$

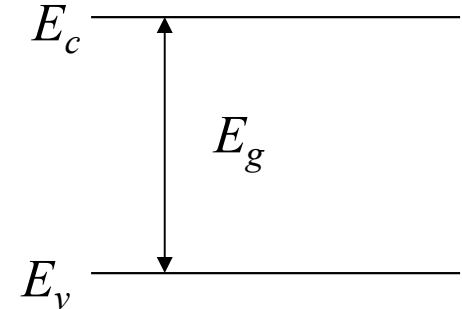
$$N_v = 2 \left( \frac{m_h^* k_B T}{2\pi \hbar^2} \right)^{3/2} = \text{Effective density of states in the valence band}$$

# Law of mass action

---

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

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



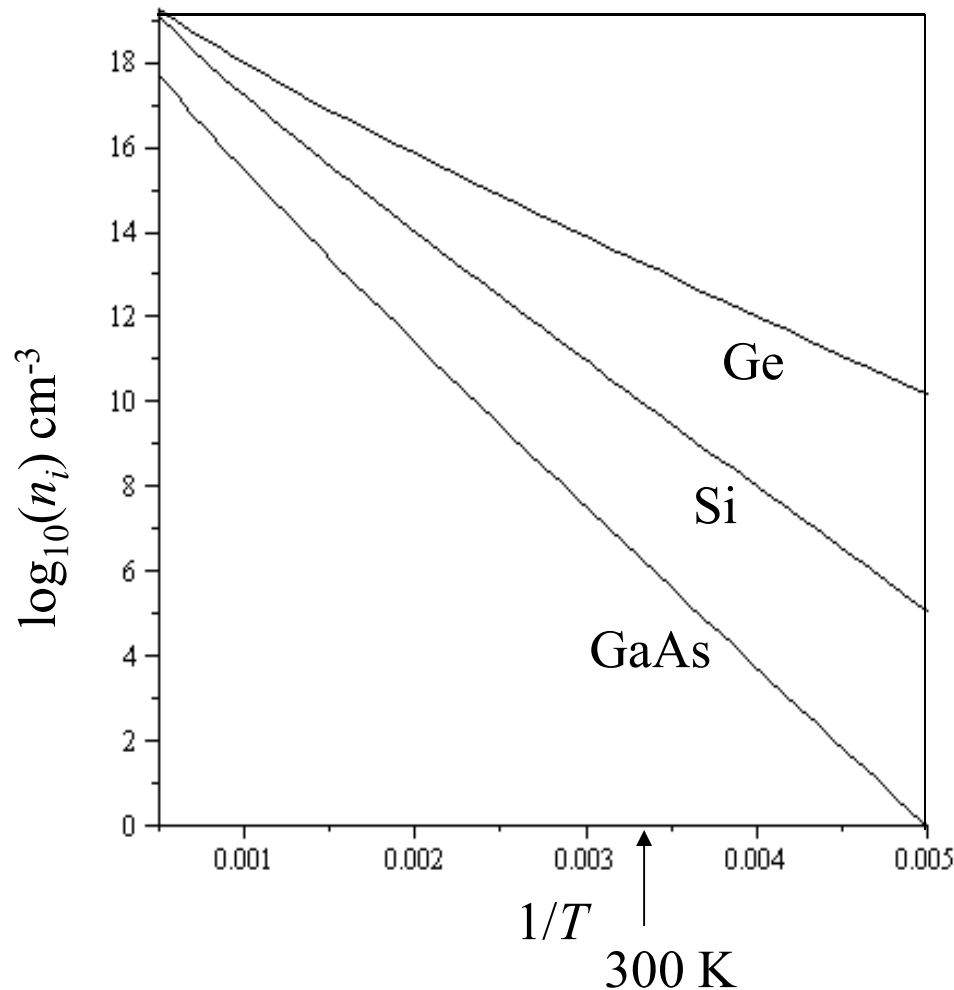
For intrinsic semiconductors (no impurities)

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

intrinsic carrier density



# Intrinsic carrier concentration



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

$$\sim 5 \times 10^{22} \text{ atoms/cm}^3$$

# Chemical potential of an intrinsic semiconductor

---

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

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

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

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

$E_c$  —————  
 $\mu$  - - - - -

$E_v$  —————

# Boltzmann approximation

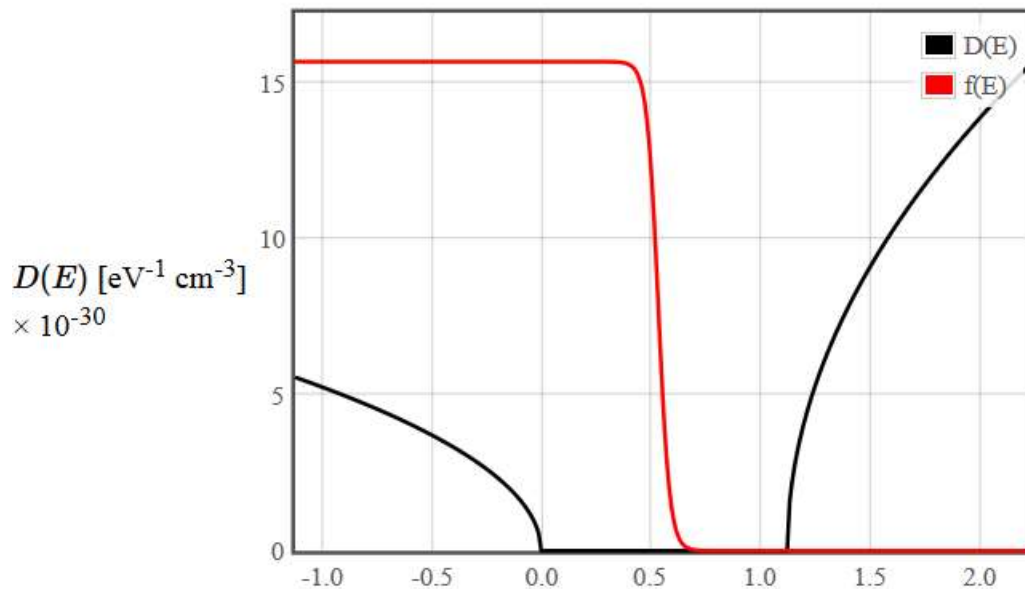
of the valence band and the bottom of the conduction band the density of states of a semiconductor can be approximated as,

$$D(E) = \begin{cases} D_v \sqrt{E_v - E}, & \text{for } E < E_v \\ 0, & \text{for } E_v < E < E_c \\ D_c \sqrt{E - E_c}, & \text{for } E_c < E \end{cases}$$

and  $D_c$  are constants that describe the form of the density of states near the band edges. Often in the literature, these constants are given in terms of the masses'  $m_h^*$  and  $m_e^*$  or the 'effective density of states at 300 K'  $N_v(300)$  and  $N_c(300)$ . The relations to  $D_v$  and  $D_c$  are,

$$D_v = \frac{(2m_h^*)^{3/2}}{2\pi^2\hbar^3} = \frac{\sqrt{\pi}N_v(300)}{2(k_B T)^{3/2}}, \quad D_c = \frac{(2m_e^*)^{3/2}}{2\pi^2\hbar^3} = \frac{\sqrt{\pi}N_c(300)}{2(k_B T)^{3/2}}.$$

Now shows the density of states of various semiconductors in this approximation. The Fermi function is plotted as well. At low energies the states are occupied. At high energies the Fermi function goes to zero and those states are unoccupied. In the limit of low temperature, the chemical potential is approximately  $\mu = E_g/2$ . As the temperature increases, the chemical potential moves towards the band with the lower density of states.



$D_c =$	<input type="text" value="1.48E31"/>	1/eV 1/cm <sup>3</sup>	Semiconductor <input type="checkbox"/> Si <input type="checkbox"/> Ge <input type="checkbox"/> GaAs <input type="checkbox"/> InAs <input type="checkbox"/> InP <input type="checkbox"/> In
$D_v =$	<input type="text" value="5.25E30"/>	1/eV 1/cm <sup>3</sup>	
$E_g =$	<input type="text" value="1.166-4.73E-4*T*T/(T+636)"/>	eV	
$T_1 =$	<input type="text" value="300"/>	K	
<input type="button" value="Replot"/>			

<http://lampx.tugraz.at/~hadley/ss1/semiconductors/boltzmann.php>

# 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.

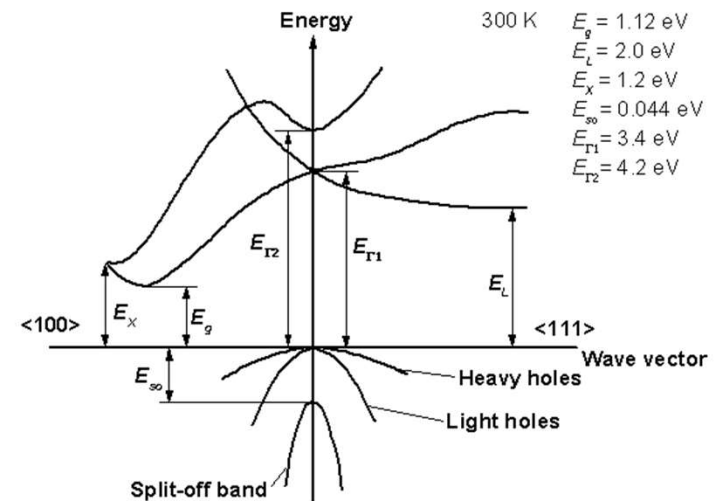
	1-d	2-d
<b>Density of states</b> $m_e^*$ and $m_h^*$ are 'density of states' effective masses	$D(E) = \begin{cases} \frac{1}{\hbar\pi} \sqrt{\frac{2m_h^*}{(E_v - E)}} & E < E_v \\ 0 & E_v < E < E_c \\ \frac{1}{\hbar\pi} \sqrt{\frac{2m_e^*}{(E - E_c)}} & E > E_c \end{cases} \quad \text{J}^{-1} \text{m}^{-1}$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

# New Semiconductor Materials. Biology systems. Characteristics and Properties

Semiconductors database	n,k	InGaAsP	Levels	Equivalentents	Bibliografic database
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## NSM Archive - Physical Properties of Semiconductors

Si	- Silicon	Ge	- Germanium
GaP	- Gallium Phosphide	GaAs	- Gallium Arsenide
InAs	- Indium Arsenide	C	- Diamond
GaSb	- Gallium Antimonide	InSb	- Indium Antimonide
InP	- Indium Phosphide	GaAs <sub>1-x</sub> Sb <sub>x</sub>	- Gallium Arsenide Antimonide
Al <sub>x</sub> Ga <sub>1-x</sub> As	- Aluminium Gallium Arsenide		
AlN	- Aluminium Nitride		
BN	- Boron Nitride		



<http://www.matprop.ru/semicond>

## Intrinsic semiconductors

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

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

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,

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

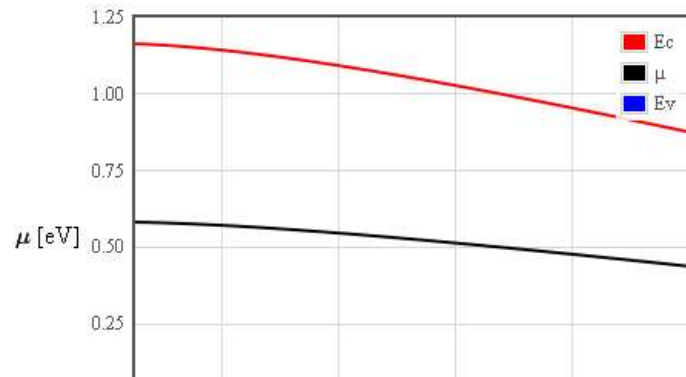
$$m_e^* = \frac{\pi\hbar^2}{300k_B} \left( \sqrt{2}N_c(300) \right)^{2/3}$$

In an intrinsic semiconductor, the density of electrons equals the density of holes,  $n = p = n_i = \sqrt{N_c \left( \frac{T}{300} \right)^{3/2} N_v \left( \frac{T}{300} \right)^{3/2} \exp\left( \frac{-E_g}{2k_B T} \right)}$ .

By setting the concentration of electrons equal to the concentration of holes, it is possible to solve for the chemical potential. The bandgap of most semiconductors is temperature dependent. The form below lets you input the temperature dependence of the bandgap. The bandgaps for some semiconductors can be loaded into the form with the buttons on the right.

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

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

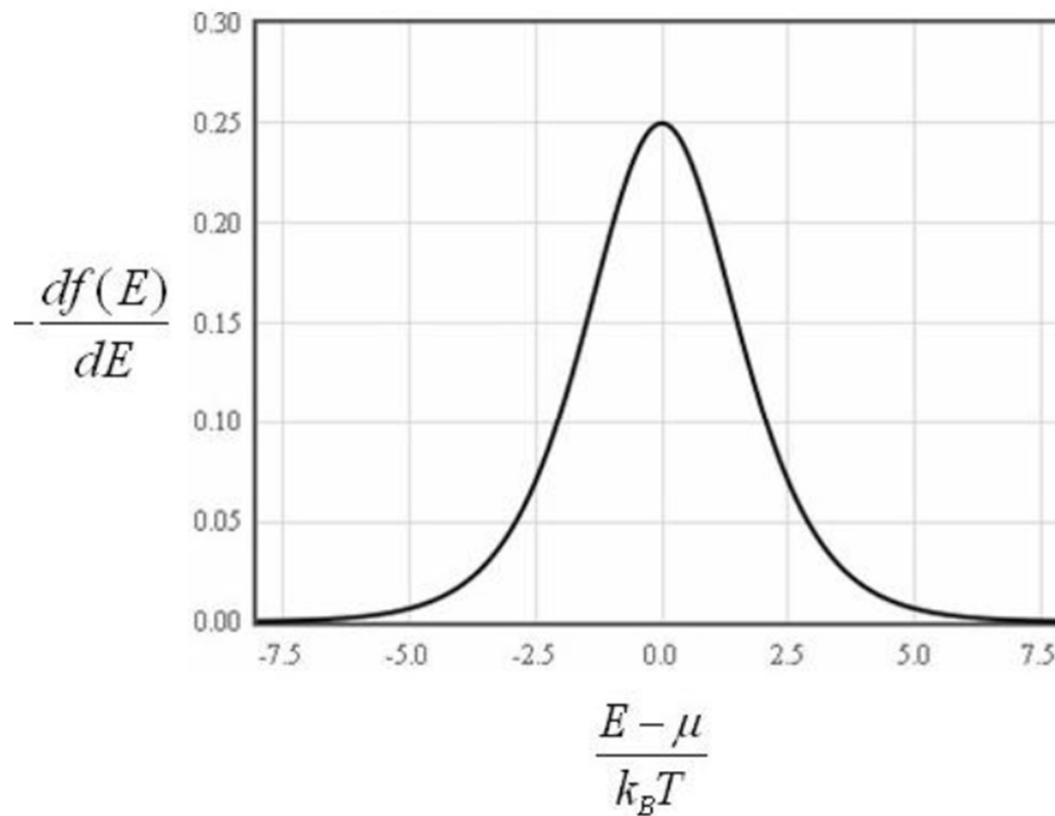


$N_c(300 \text{ K}) =$	<input type="text" value="2.78E19"/>	1/cm <sup>3</sup>	Semiconductor <input type="button" value="Si"/> <input type="button" value="Ge"/> <input type="button" value="GaAs"/>
$N_v(300 \text{ K}) =$	<input type="text" value="9.84E18"/>	1/cm <sup>3</sup>	
$E_g =$	<input type="text" value="1.166-4.73E-4*T*(T+636)"/>	eV	
$T_1 =$	<input type="text" value="50"/>	K	
$T_2 =$	<input type="text" value="1000"/>	K	
<input type="button" value="Replot"/>			

## Density of states → internal energy density for electrons in metals

The internal energy density  $u$  is the integral of the energy  $E$  times the density of states  $D(E)$  times the probability that those states are occupied. The occupation probability is given by the Fermi function  $f(E)$ .

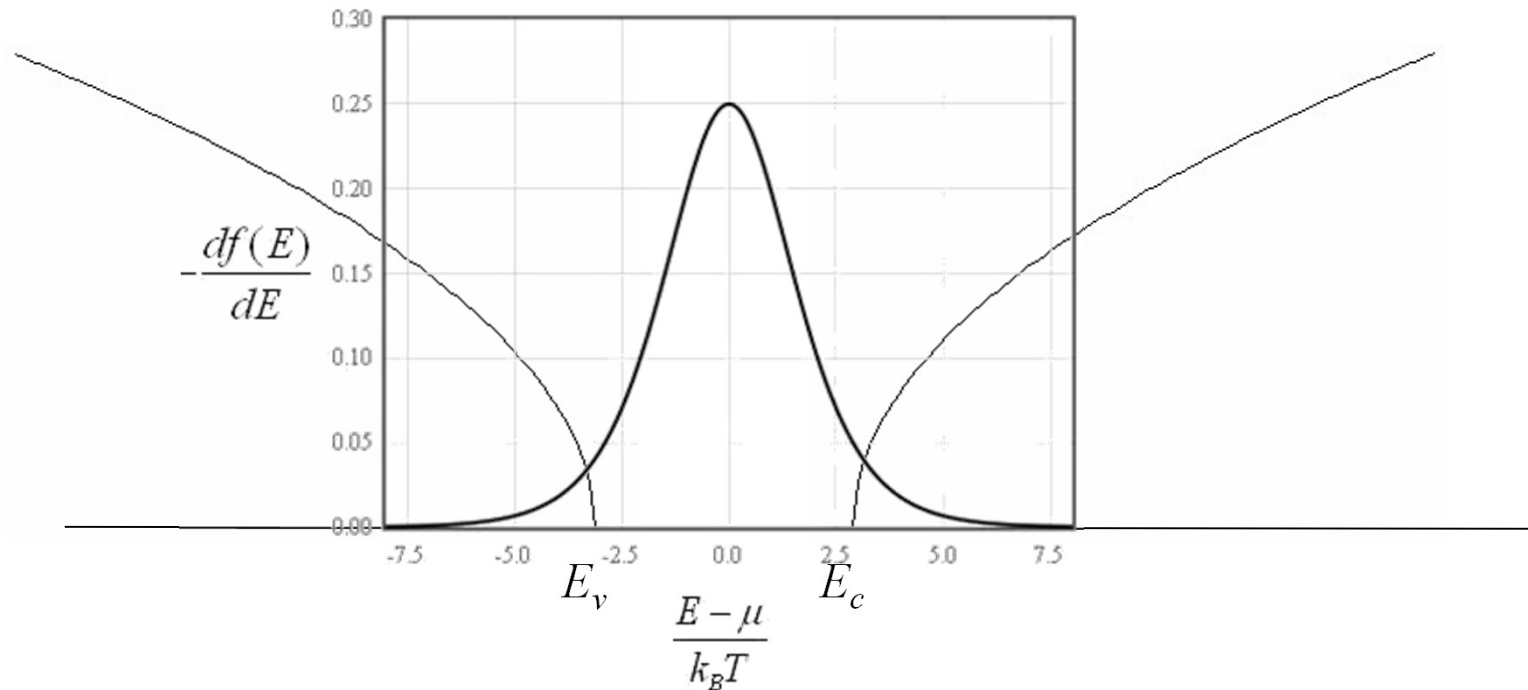
$$u = \int_{-\infty}^{\infty} ED(E) f(E) dE = \int_{-\infty}^{\infty} \frac{ED(E) dE}{\exp\left(\frac{E - \mu}{k_B T}\right) + 1}$$



<http://lampx.tugraz.at/~hadley/ss1/materials/thermo/dos2u.html>

# Narrow bandgap semiconductors

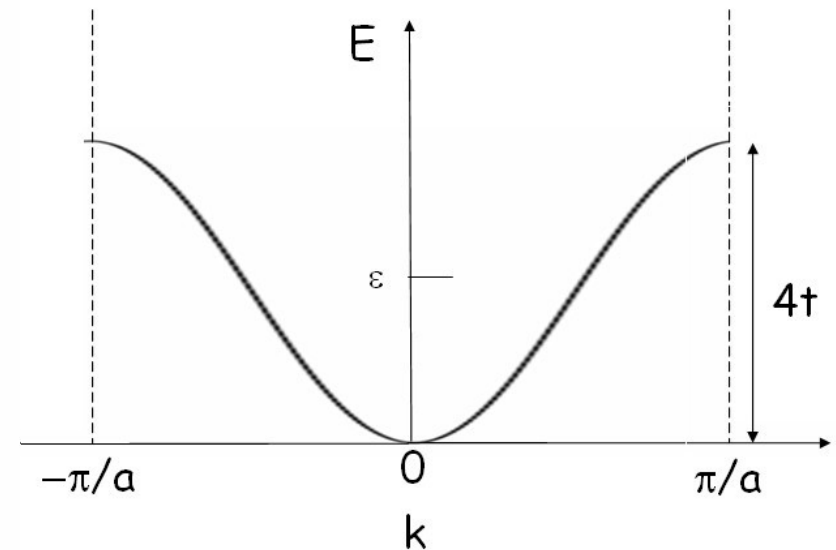
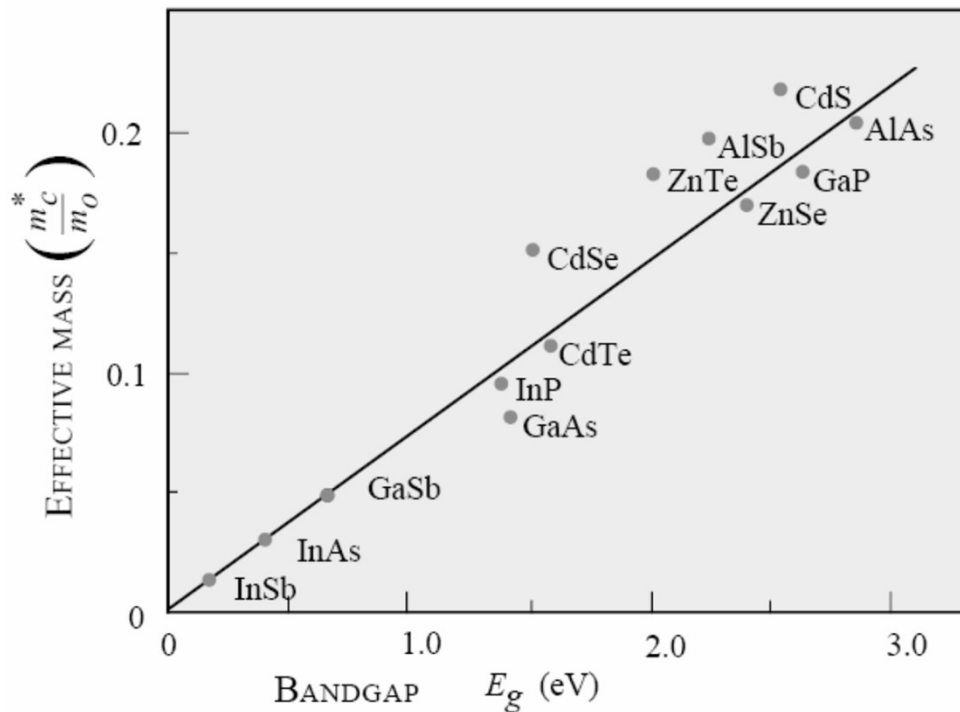
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Use the programs for metals for small bandgap semiconductors.



# Large gap -> large effective mass



$$E_k = \varepsilon - 2t \cos(ka)$$

$$m^* = \frac{\hbar^2}{\frac{d^2 E}{dk^2}}$$

$$\frac{d^2 E}{dk^2} = 2ta^2$$

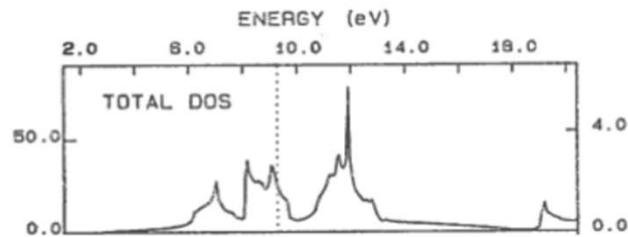
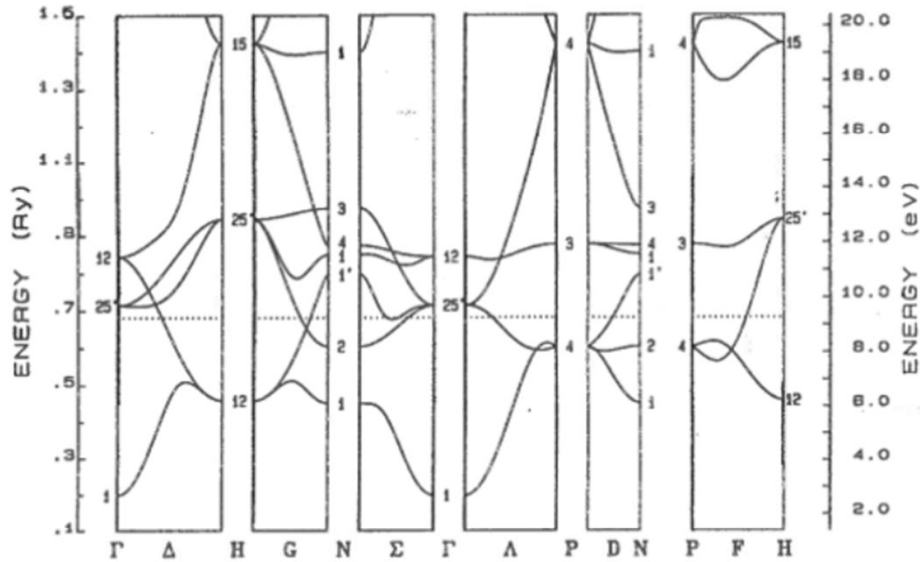
$$m^* \propto \frac{1}{t}$$

narrow bands -> large effective mass

## Metal, semiconductor, insulator

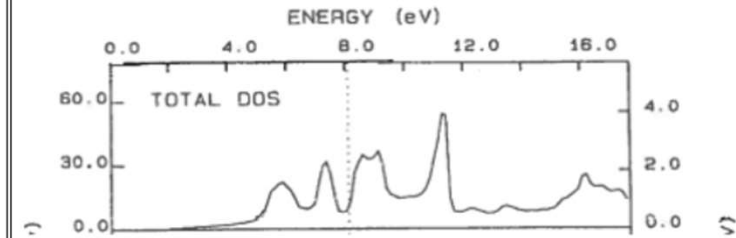
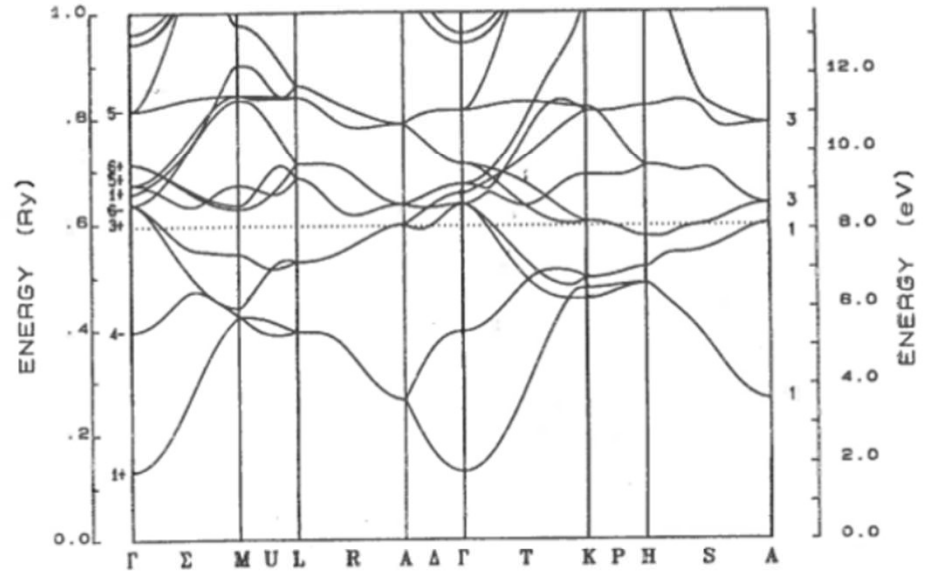
Classify these materials as metals, semi-metals, semiconductors, or insulators. The dotted line shows the highest occupied electron state. For semiconductors and insulators, state if the band gap is direct or indirect.

(a)



(c)

(b)



(d)