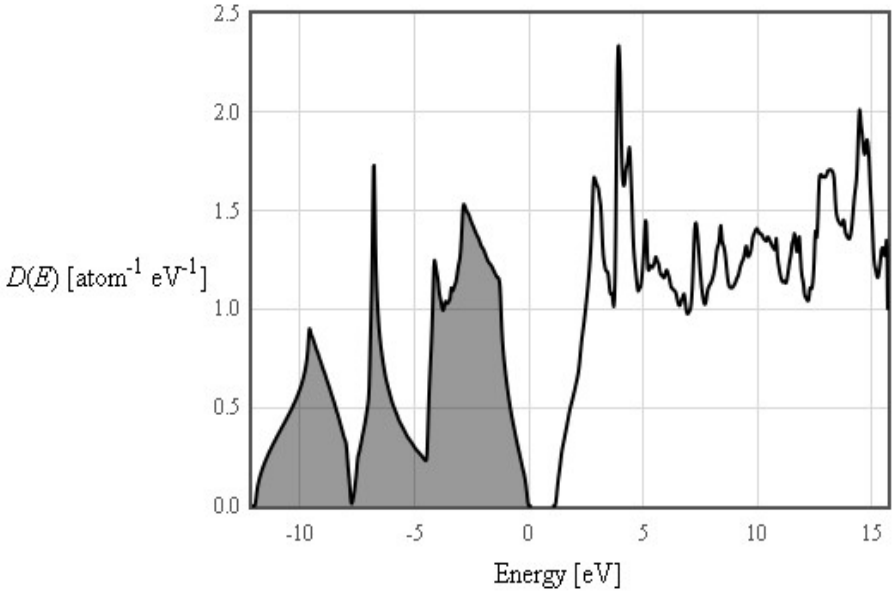
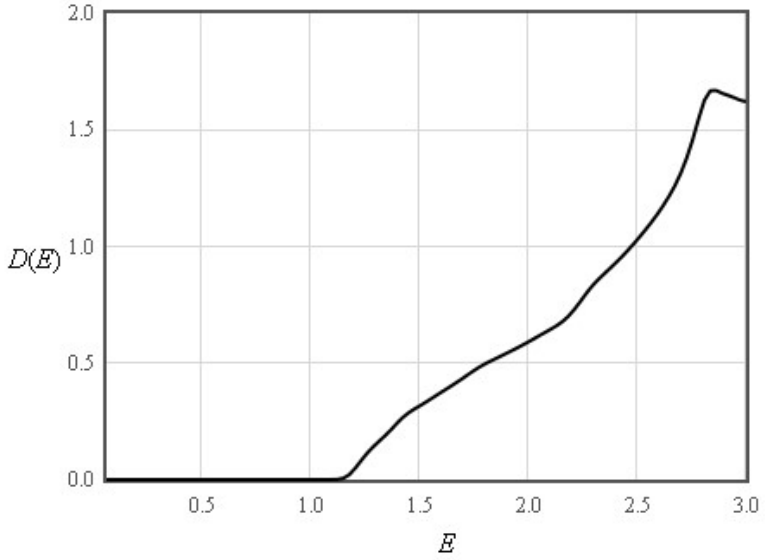
Electrons

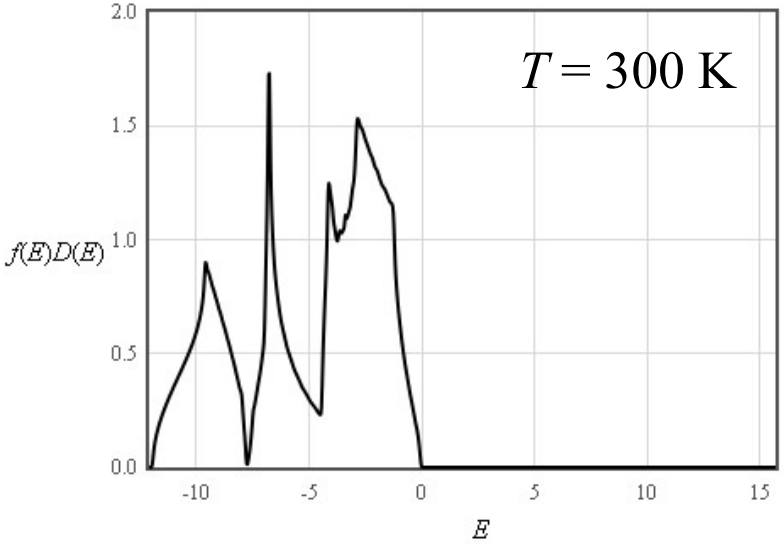
Exam

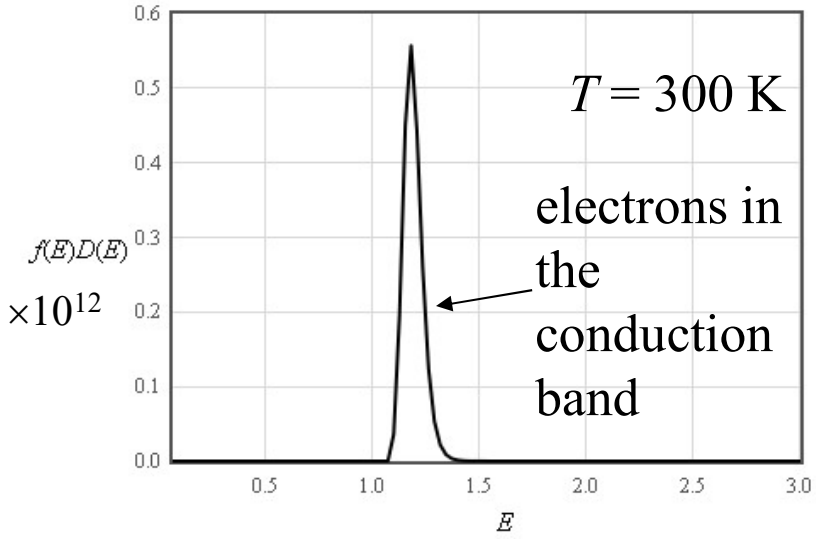
One A4 handwritten notes
One hour
Like the exams online

Silicon density of states









Boltzmann Approximation

Density of electrons in the conduction band

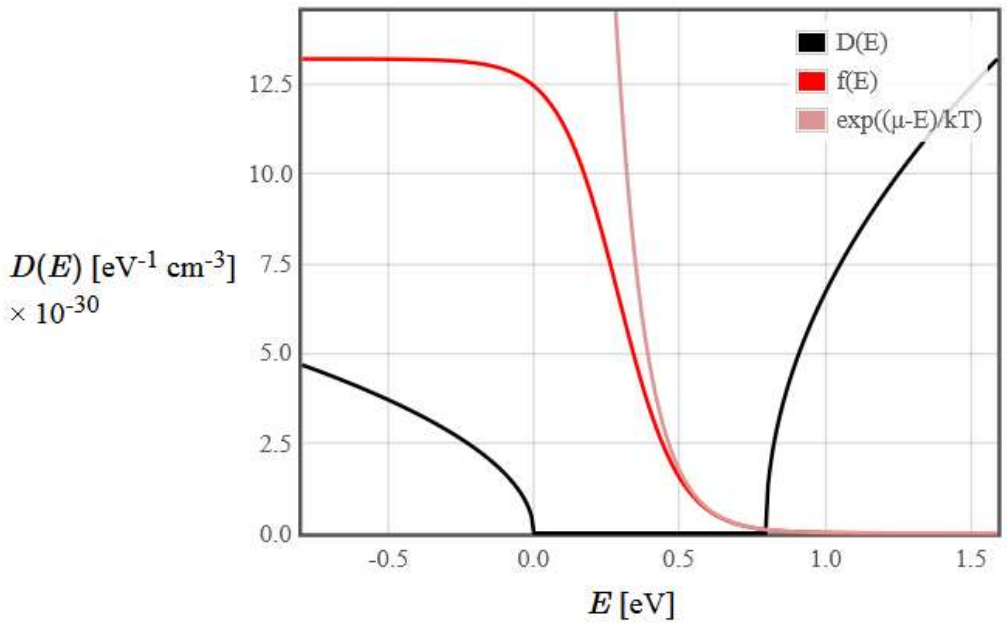
The free electron density of states is modified by the effective mass.

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

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

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

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

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

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

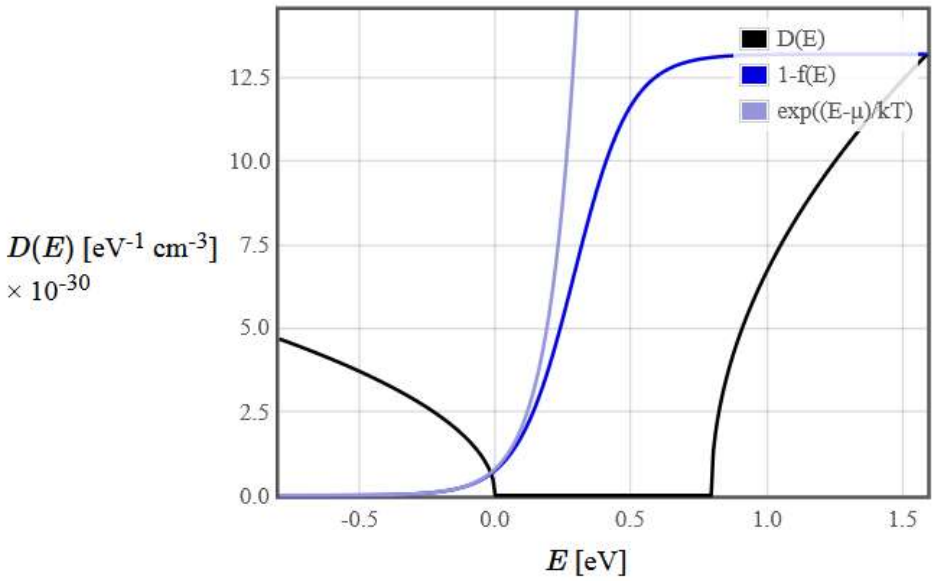
$$\boxed{n = N_c(T) \exp\left(\frac{\mu - E_c}{k_B T}\right)} = \frac{\sqrt{\pi} D_c}{2} (k_B T)^{3/2} \exp\left(\frac{\mu - E_c}{k_B T}\right)$$

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

Density of holes in the valence band

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

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

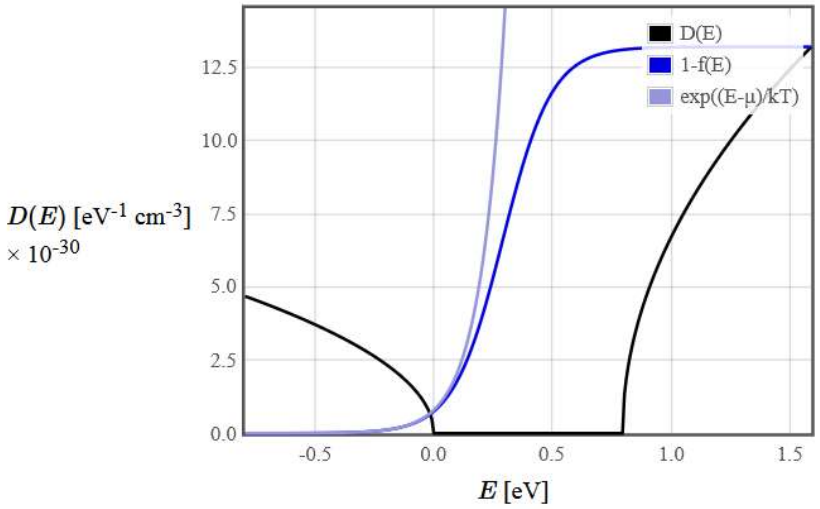


Boltzmann approximation

$\mu - E_v > 3k_B T$

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

Density of holes in the valence band



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

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

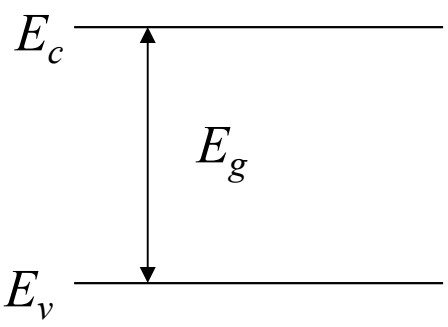
$$N_v = 2\left(\frac{m_h^* k_B T}{2\pi\hbar^2}\right)^{3/2}$$

= Effective density of states in the valence band

Law of mass action

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

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

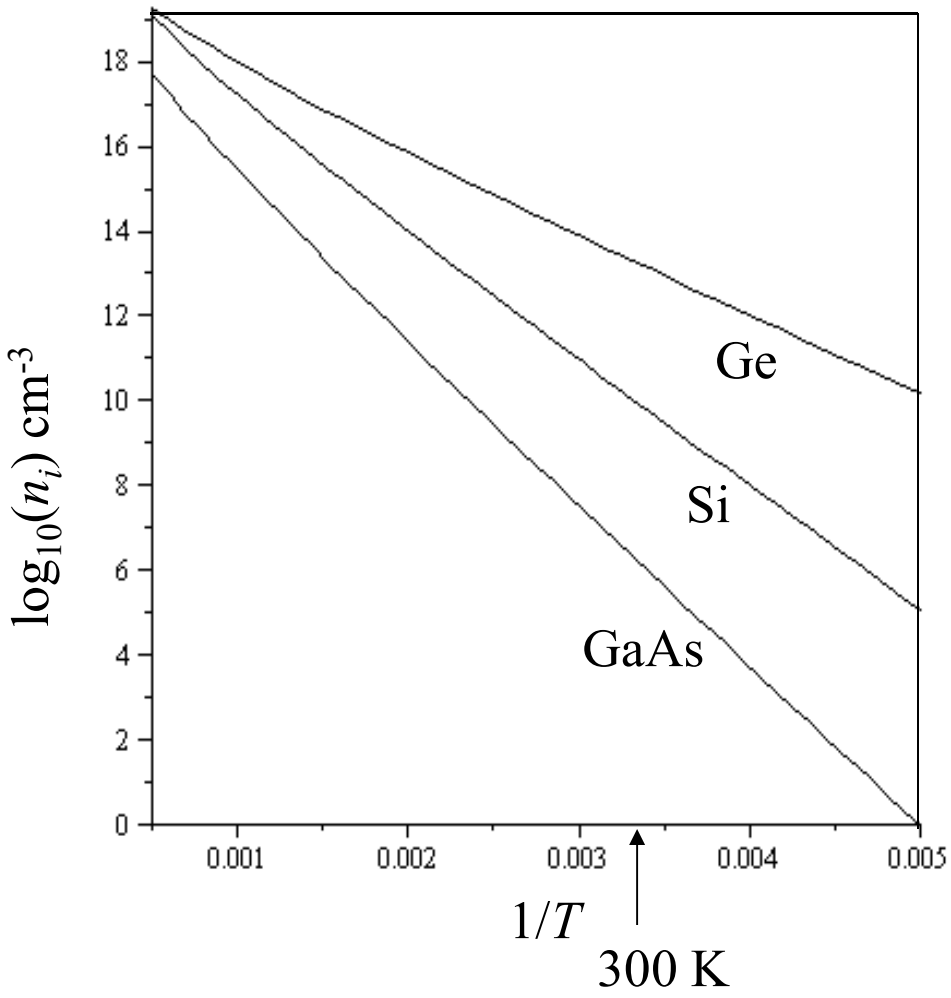


For intrinsic semiconductors (no impurities)

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

intrinsic carrier density

Intrinsic carrier concentration



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

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

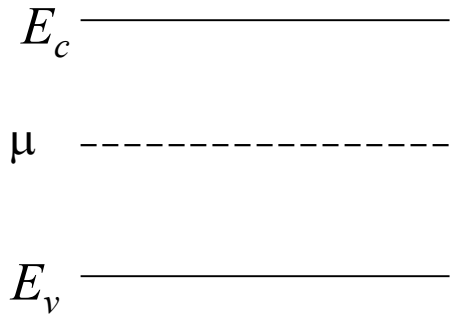
Chemical potential of an intrinsic semiconductor

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

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

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

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



Boltzmann approximation

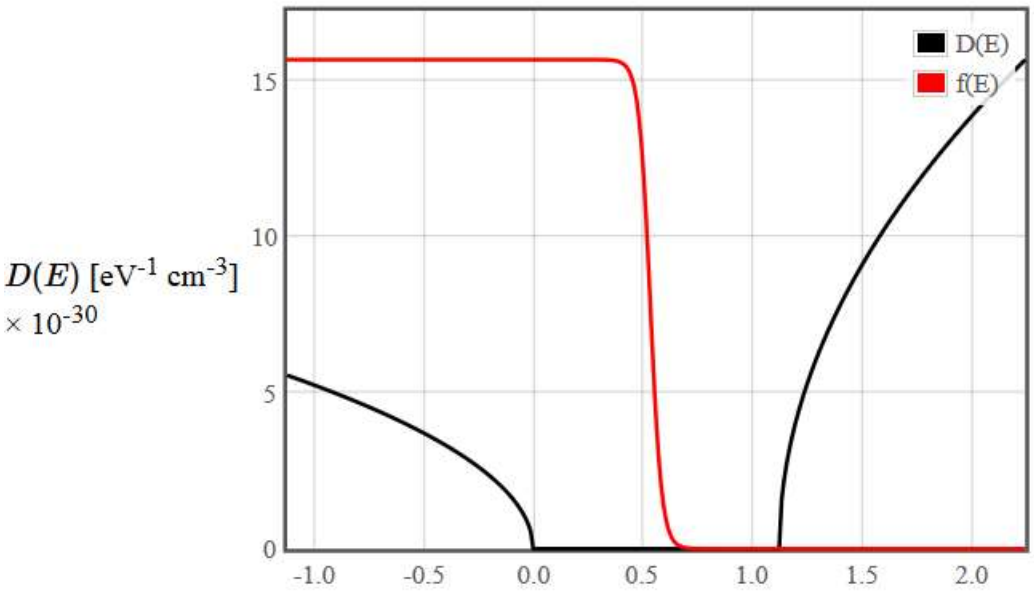
of the valence band and the bottom of the conduction band the density of states of a semiconductor can be approximated as,

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

ıd 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 sses' 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,

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

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



D_c =	1.48E31	1/eV 1/cm³
D_v =	5.25E30	1/eV 1/cm³
E_g =	1.166-4.73E-4*T*T/(T+636)	eV
T_1 =	300	K

Replot

Semiconductor

Si | Ge | GaAs | InAs | InP | In

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 where calculated in the Boltzmann approximation where it is assumed that the chemical potential lies in the band gap more than $3k_BT$ 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	$D(E) = \begin{cases} \frac{1}{\hbar\pi}\sqrt{\frac{2m_h^*}{(E_v - E)}} & E < E_v \\ 0 & E_v < E < E_c \\ \frac{1}{\hbar\pi}\sqrt{\frac{2m_e^*}{(E - E_c)}} & E > E_c \end{cases}$ J^{-1} m^{-1}	$D(E) = \begin{cases} \frac{m_h^*}{\hbar^2\pi}H(E_v - E) & E < E_v \\ 0 & E_v < E < E_c \\ \frac{m_e^*}{\hbar^2\pi}H(E - E_c) & E > E_c \end{cases}$ J^{-1} m^{-2} $H(x) = 0$ for $x < 0$ and $H(x) = 1$ for $x > 0$
Density of states N_V and N_C are the effective densities of states	$D(E) = \begin{cases} N_v(300)\sqrt{\frac{2}{300\pi k_B(E_v - E)}} & E < E_v \\ 0 & E_v < E < E_c \\ N_c(300)\sqrt{\frac{2}{300\pi k_B(E - E_c)}} & E > E_c \end{cases}$ J^{-1} m^{-1}	$D(E) = \begin{cases} \frac{N_v(300)}{300k_B}H(E_v - E) & E < E_v \\ 0 & E_v < E < E_c \\ \frac{N_c(300)}{300k_B}H(E - E_c) & E > E_c \end{cases}$ J^{-1} m^{-2}
Density of electrons in the conduction band $n = \int_{E_c}^{\infty} D(E)f(E)dE$	$n = \sqrt{\frac{m_e^* k_B T}{\hbar^2\pi}}\exp\left(\frac{\mu - E_c}{k_B T}\right)$ m^{-1} $= N_c \exp\left(\frac{\mu - E_c}{k_B T}\right)$	$n = \frac{m_e^* k_B T}{\hbar^2\pi}\exp\left(\frac{\mu - E_c}{k_B T}\right)$ m^{-2} $= N_c \exp\left(\frac{\mu - E_c}{k_B T}\right)$
Density of holes in the valence band $p = \int_{-\infty}^{E_v} D(E)(1 - f(E))dE$	$p = \sqrt{\frac{m_h^* k_B T}{\hbar^2\pi}}\exp\left(\frac{E_v - \mu}{k_B T}\right)$ m^{-1} $= N_v \exp\left(\frac{\mu - E_c}{k_B T}\right)$	$p = \frac{m_h^* k_B T}{\hbar^2\pi}\exp\left(\frac{E_v - \mu}{k_B T}\right)$ m^{-2} $= N_v \exp\left(\frac{\mu - E_c}{k_B T}\right)$

Intrinsic semiconductors

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

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

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,

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

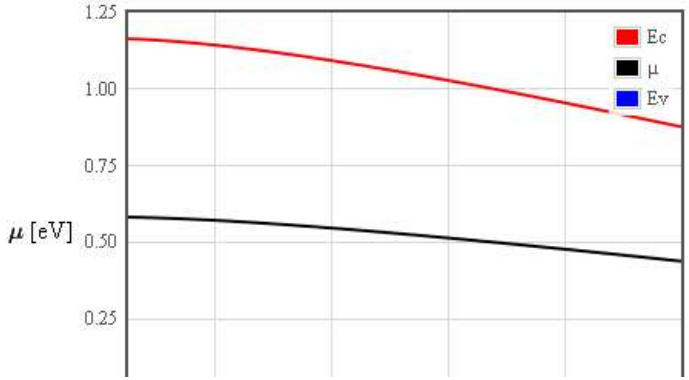
$$m_e^* = \frac{\pi\hbar^2}{300k_B}\left(\sqrt{2}N_c(300)\right)^{2/3}$$

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

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 dependance of the bandgap. The bandgaps for some semiconductors can be loaded into the form with the buttons on the right.

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

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



$N_c(300\text{ K}) =$ 2.78E19 1/cm³

$N_v(300\text{ K}) =$ 9.84E18 1/cm³

$E_g =$ 1.166-4.73E-4*T*T/(T+636) eV

$T_1 =$ 50 K

$T_2 =$ 1000 K

Replot

Semiconductor

Si Ge GaAs

http://lamp.tu-graz.ac.at/~hadley/ss1/semiconductors/intrinsic.php

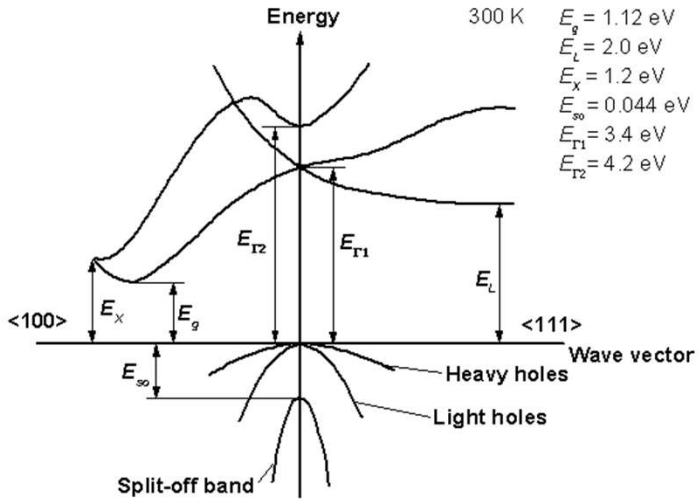
New Semiconductor Materials. Biology systems.
Characteristics and Properties

Semiconductors n,k

database InGaAsP Levels Equivalents Bibliografic database

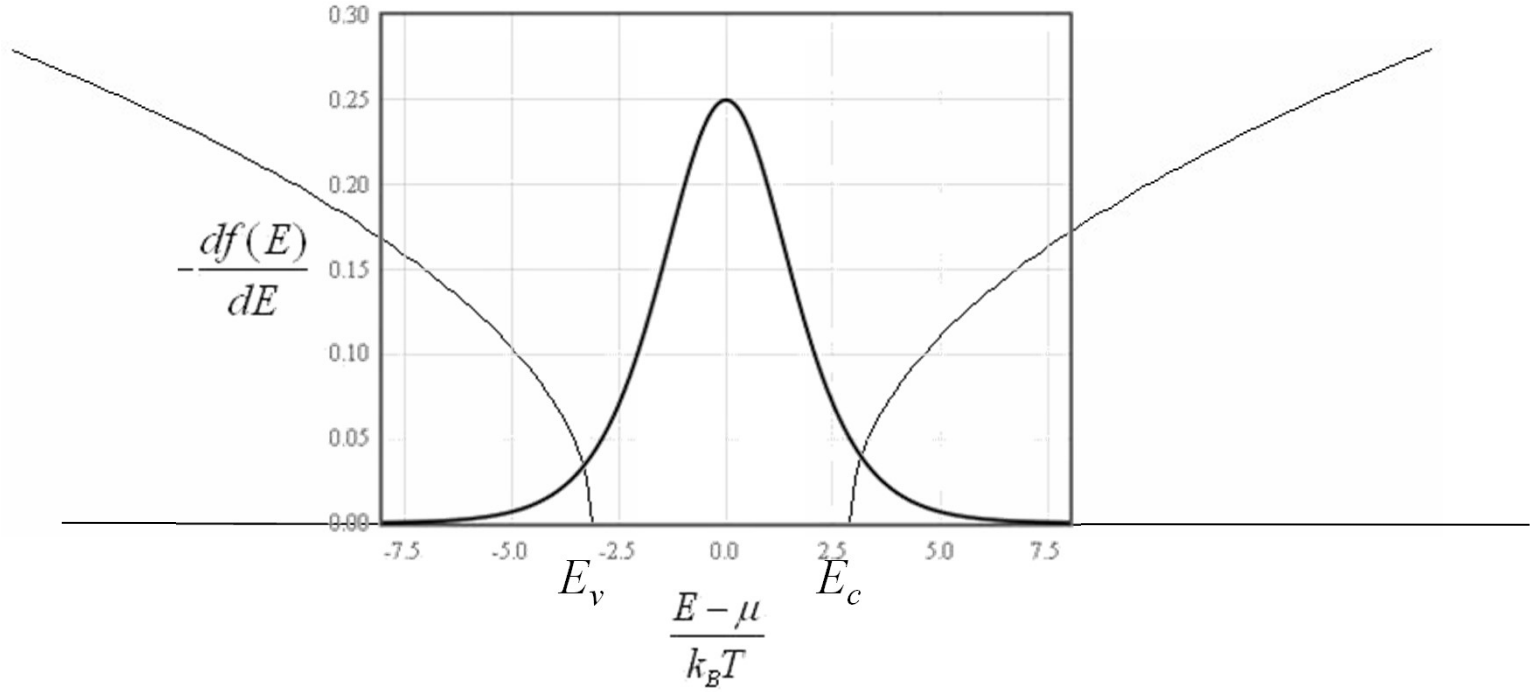
NSM Archive - Physical Properties of Semiconductors

Si	- Silicon	Ge	- Germanium
GaP	- Gallium Phosphide	GaAs	- Gallium Arsenide
InAs	- Indium Arsenide	C	- Diamond
GaSb	- Gallium Antimonide	InSb	- Indium Antimonide
InP	- Indium Phosphide	$GaAs_{1-x}Sb_x$	- Gallium Arsenide Antimonide
$Al_xGa_{1-x}As$	- Aluminium Gallium Arsenide		
AlN	- Aluminium Nitride		
BN	- Boron Nitride		



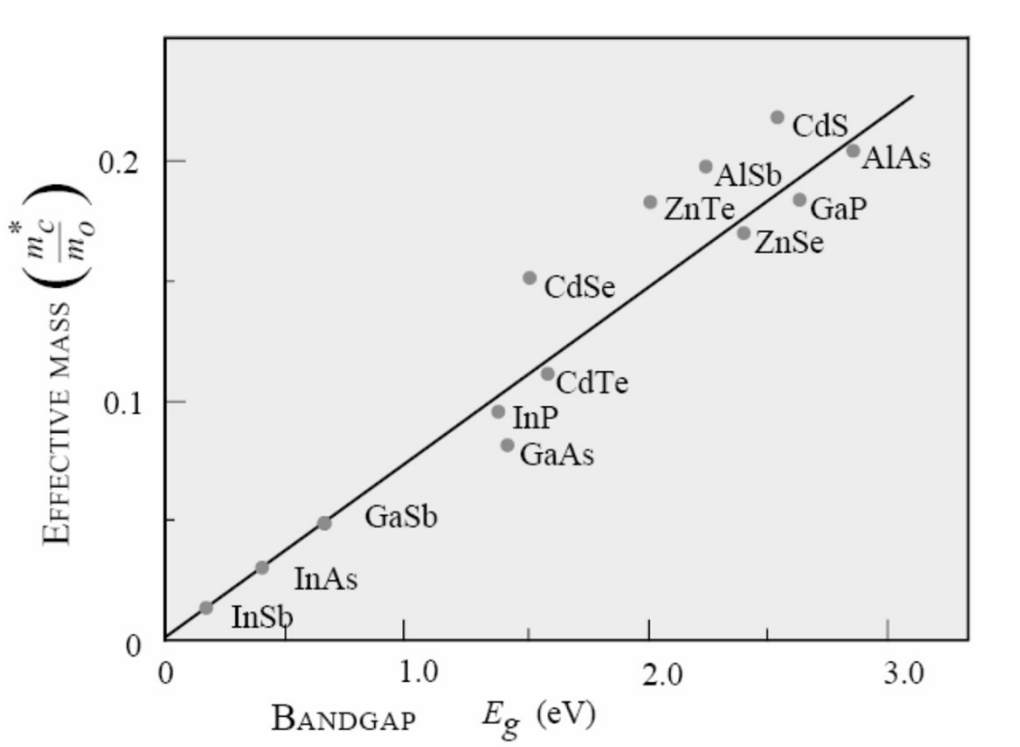
http://www.matprop.ru/semicond

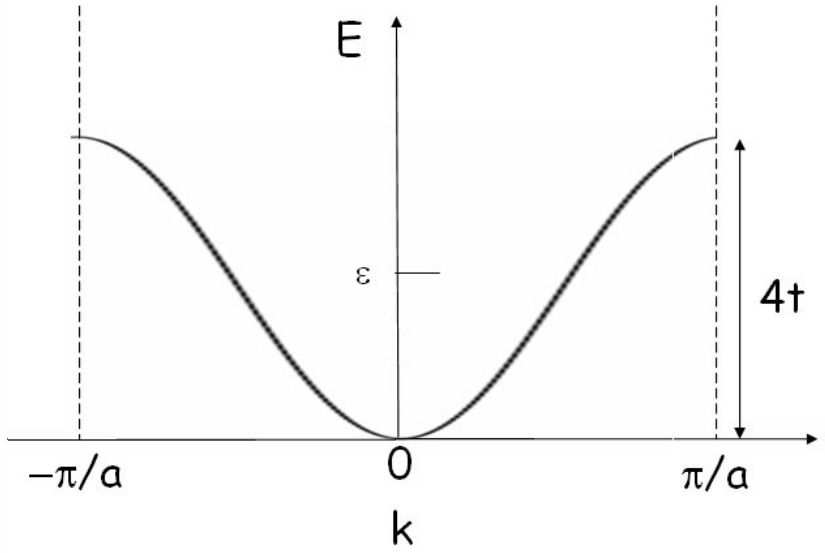
Narrow bandgap semiconductors



Use the programs for metals for small bandgap semiconductors.

Large gap -> large effective mass





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

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

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

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

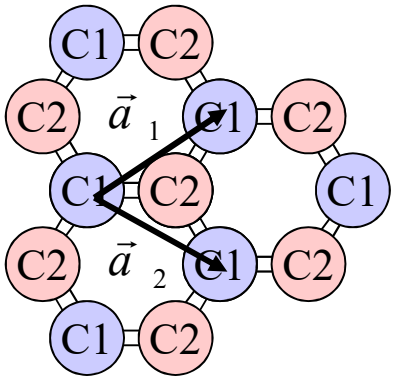
narrow bands -> large effective mass

Some interesting materials

polytypes

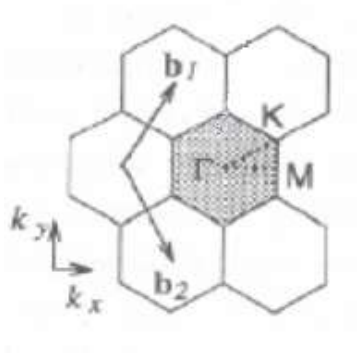
Different polytypes ⇨ Different properties

Graphene



$$\vec{a}_1 = \frac{\sqrt{3}}{2} a\hat{x} + \frac{1}{2} a\hat{y}$$

$$\vec{a}_2 = \frac{\sqrt{3}}{2} a\hat{x} - \frac{1}{2} a\hat{y}$$

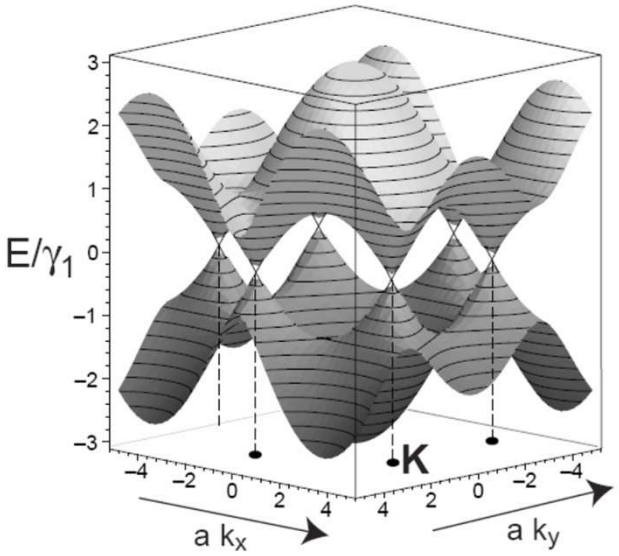


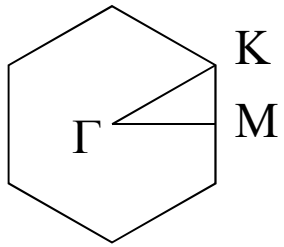
Two atoms per unit cell

Graphene has an unusual dispersion relation in the vicinity of the Fermi energy.

Tight binding, graphene

$$E = \varepsilon \pm t\sqrt{1 + 4\cos\left(\frac{\sqrt{3}k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right) + 4\cos^2\left(\frac{k_y a}{2}\right)}$$



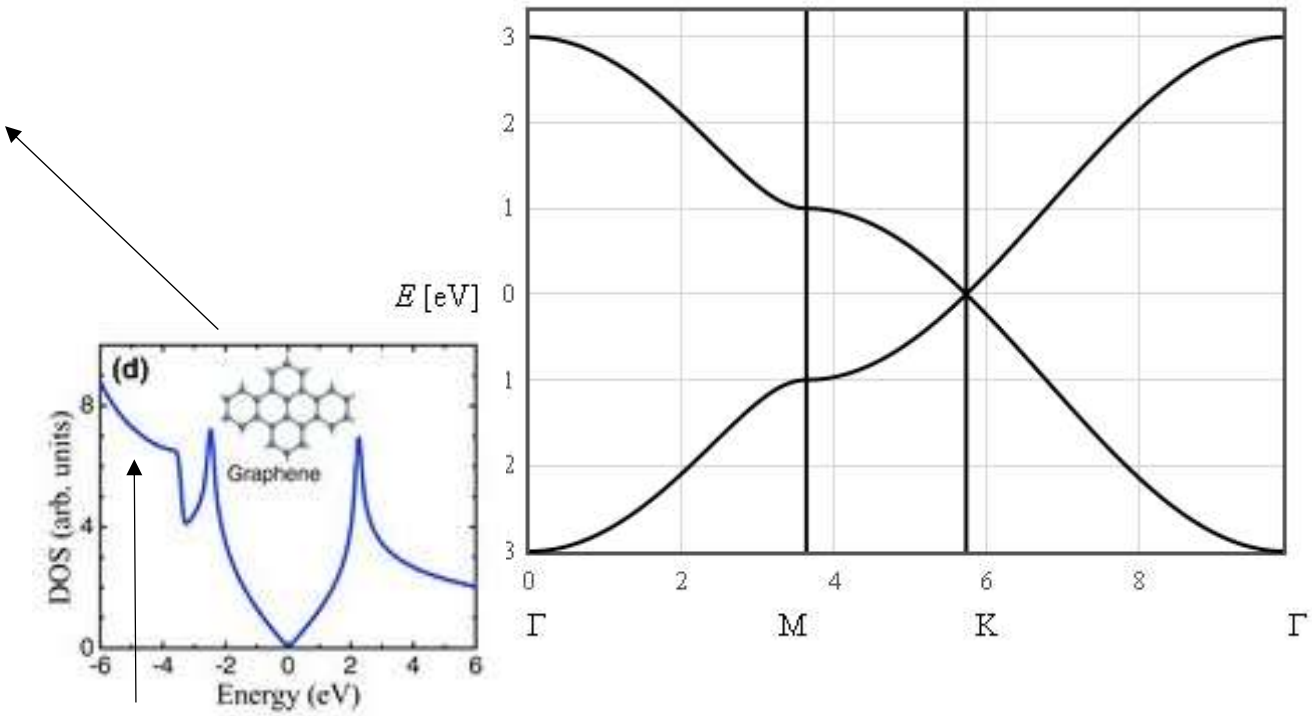


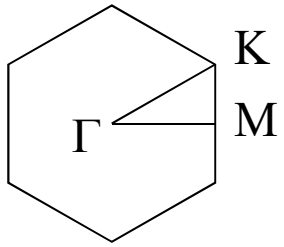
www.physics.umd.edu/courses/Phys732/hdrew/spring07/Schoenenberger%20tutorial%20on%20CNT%20bands.pdf

http://onlinelibrary.wiley.com/doi/10.1002/adfm.201101241/full

Tight binding dispersion relation for graphene

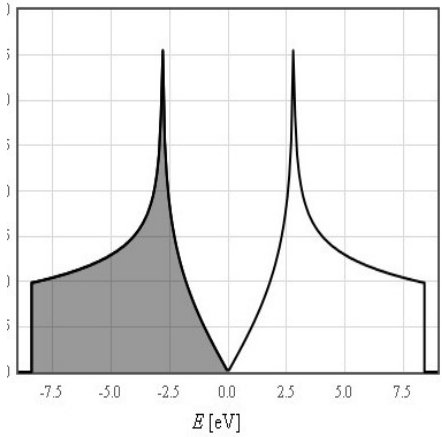
$$E = \varepsilon \pm t\sqrt{1+4\cos\left(\frac{\sqrt{3}k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right)+4\cos^2\left(\frac{k_y a}{2}\right)}$$





ε = 0 [eV]
t = 2.8 [eV]
Replot E(k)

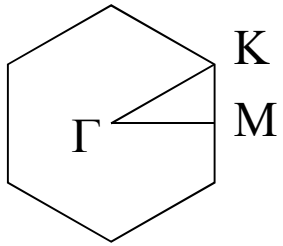
Another band is included here.

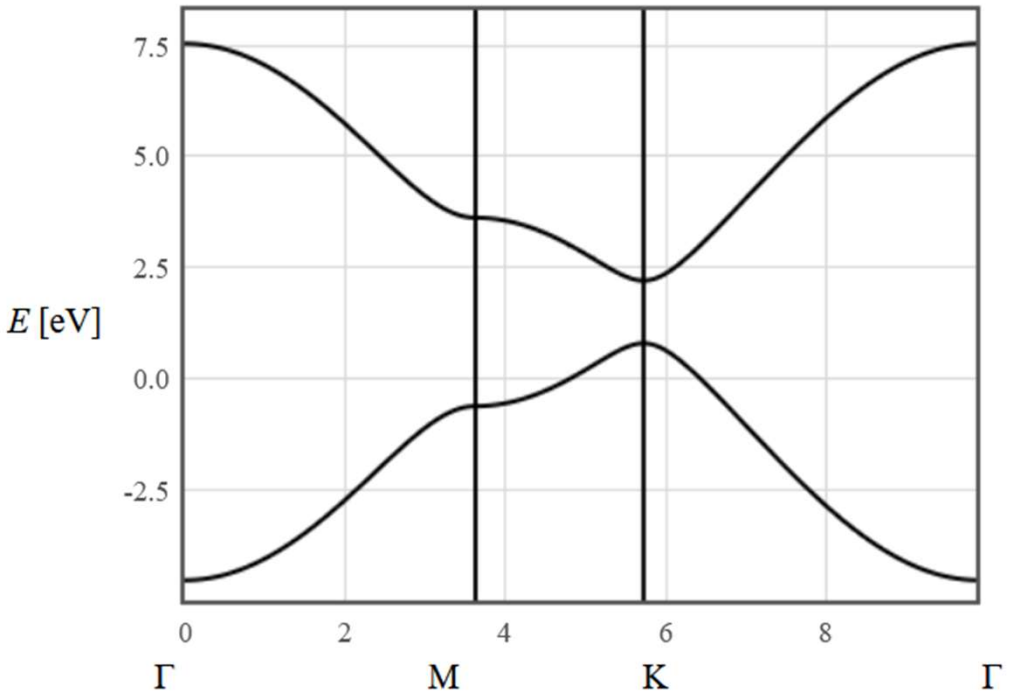


http://lamp.tu-graz.ac.at/~hadley/ss1/bands/tbtable/dispgraphene.html

2-D boron nitride

$$E = \frac{\varepsilon_1 + \varepsilon_2}{2} \pm \sqrt{\frac{(\varepsilon_1 - \varepsilon_2)^2}{2} + 4t^2 \left(\cos\left(\frac{\sqrt{3}k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right) + \cos^2\left(\frac{k_y a}{2}\right) + \frac{1}{4} \right)}$$





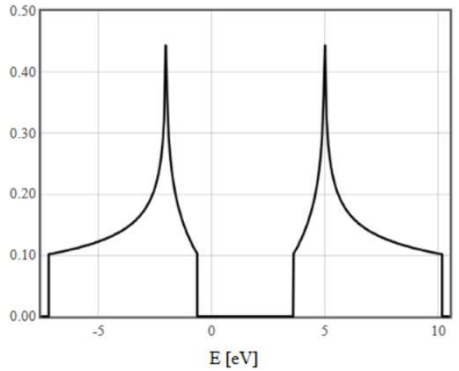
2.8

ε_1 = 2 [eV]

ε_2 = 1 [eV]

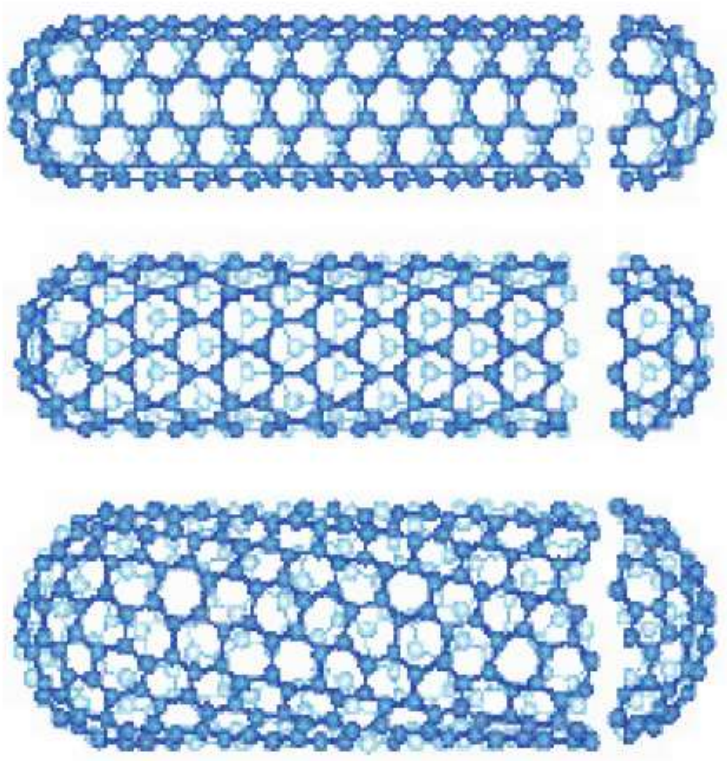
t = 2 [eV]

Replot E(k)



http://lampz.tugraz.at/~hadley/ss1/bands/tbtable/dispbn.html

Carbon nanotubes - rolled up graphene



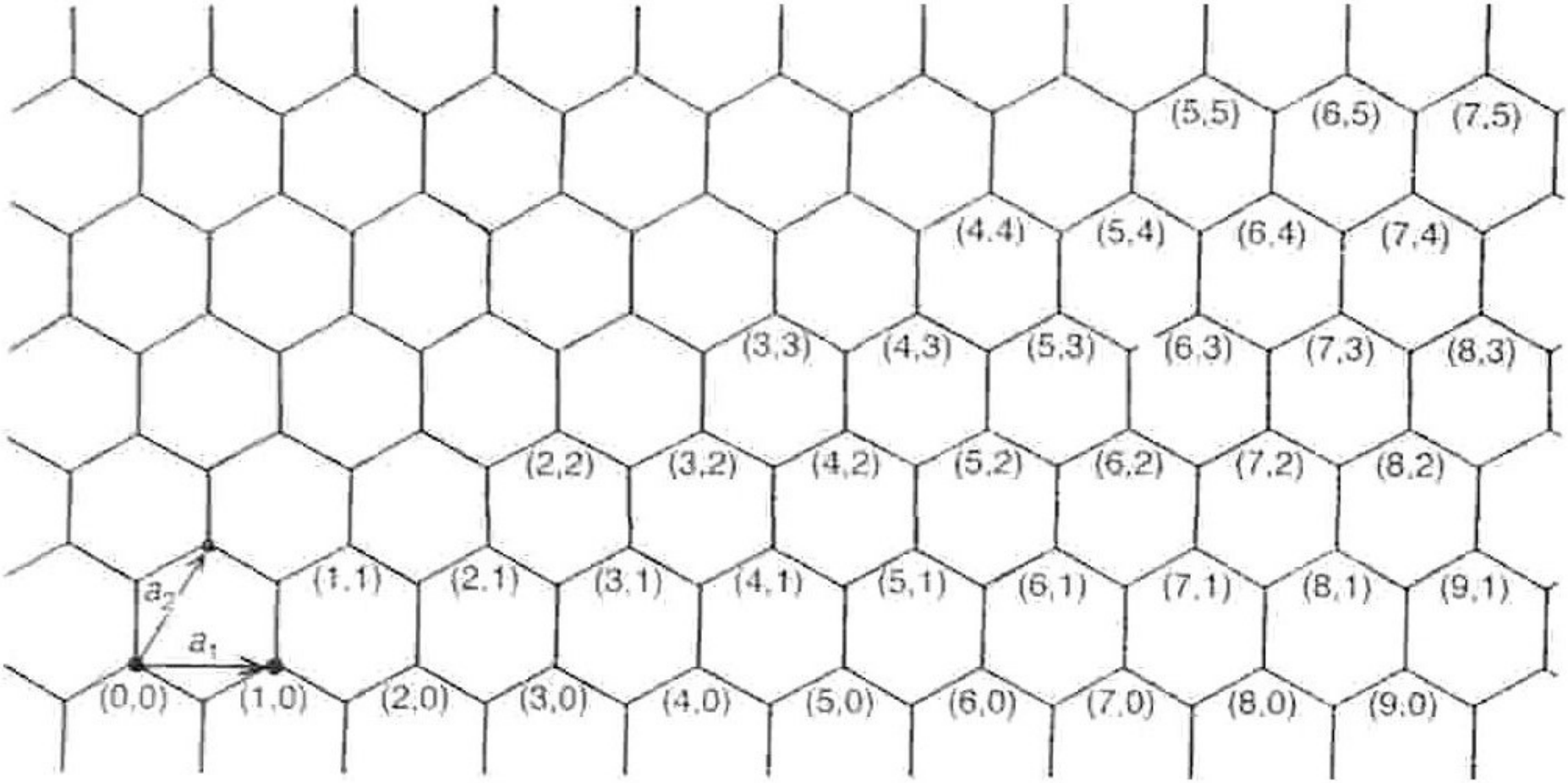
armchair

zig-zag

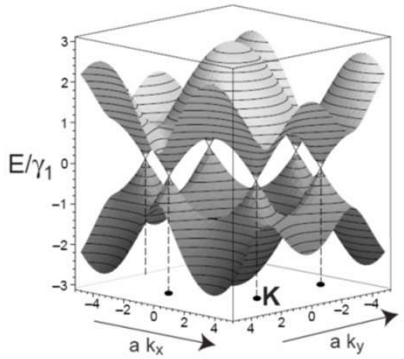
chiral

www.physics.umd.edu/courses/Phys732/hdrew/spring07/Schoenenberger%20tutorial%20on%20CNT%20bands.pdf

(*m*,*n*) notation

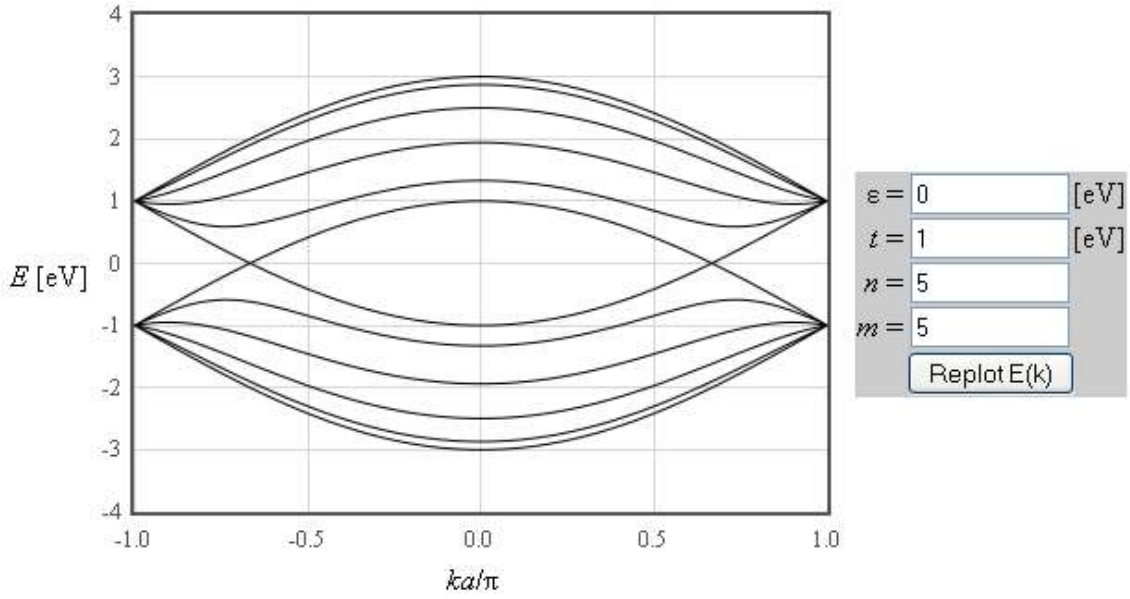


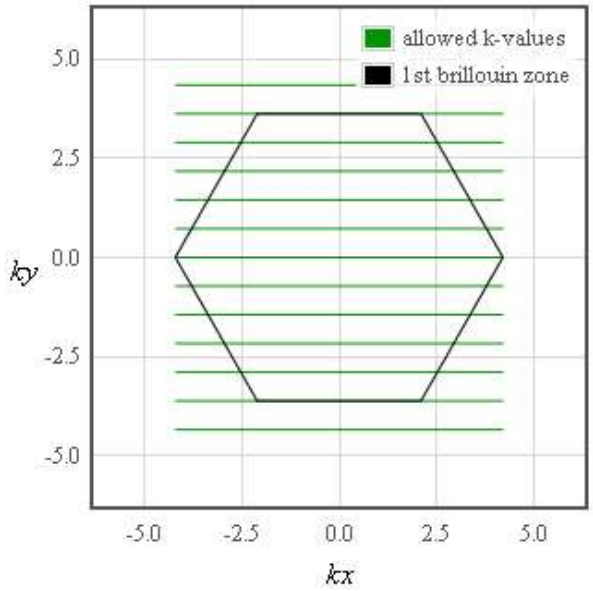
http://www.personal.rdg.ac.uk/~scsharip/tubes.htm



Carbon nanotubes

$$E = \varepsilon \pm t\sqrt{1 + 4\cos\left(\frac{\sqrt{3}k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right) + 4\cos^2\left(\frac{k_y a}{2}\right)}$$

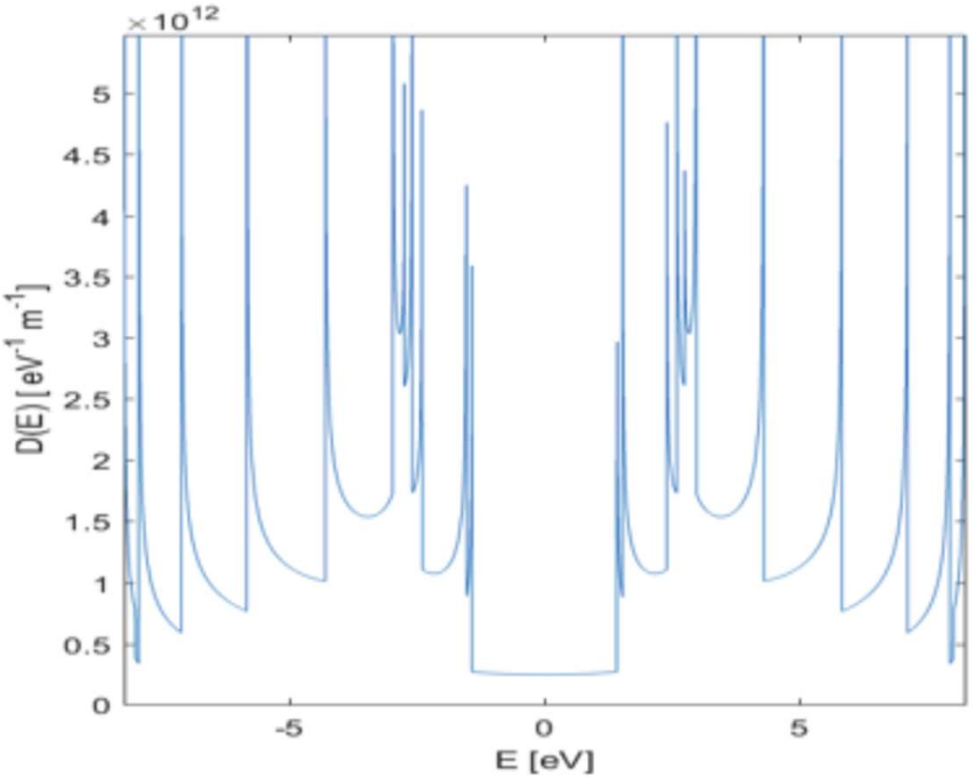




metallic (5,5) armchair tube

http://lamp.tu-graz.ac.at/~hadley/ss1/bands/tbtable/CNTs.html

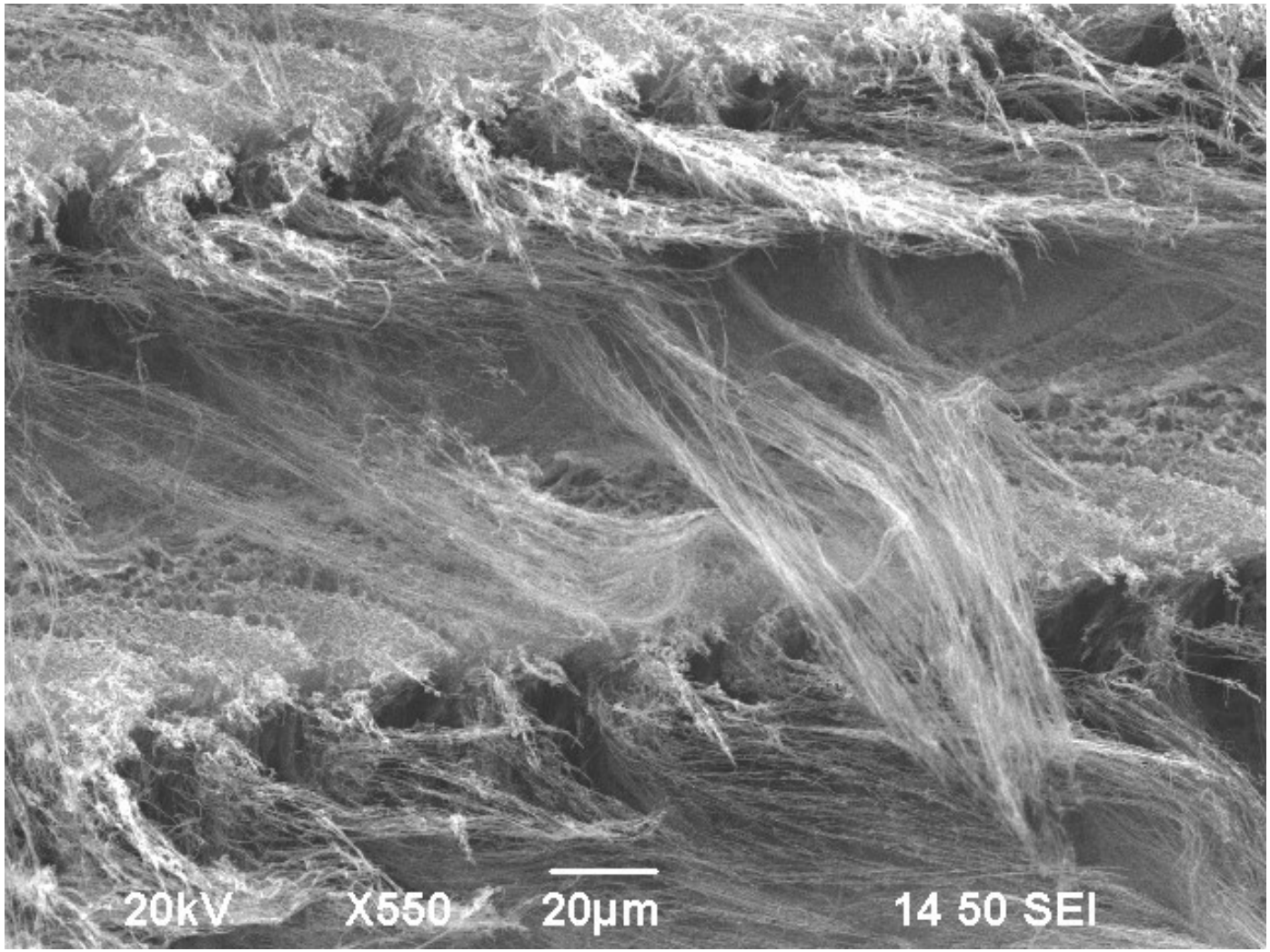
Electronic density of states of carbon nanotubes



(3,0)	(4,0)	(5,0)	(6,0)	(7,0)	(8,0)	(9,0)	(10,0)	(11,0)	(12,0)	(13,0)	(14,0)	(15,0)
(3,1)	(4,1)	(5,1)	(6,1)	(7,1)	(8,1)	(9,1)	(10,1)	(11,1)	(12,1)	(13,1)	(14,1)	(15,1)
(3,2)	(4,2)	(5,2)	(6,2)	(7,2)	(8,2)	(9,2)	(10,2)	(11,2)	(12,2)	(13,2)	(14,2)	(15,2)
(3,3)	(4,3)	(5,3)	(6,3)	(7,3)	(8,3)	(9,3)	(10,3)	(11,3)	(12,3)	(13,3)	(14,3)	(15,3)

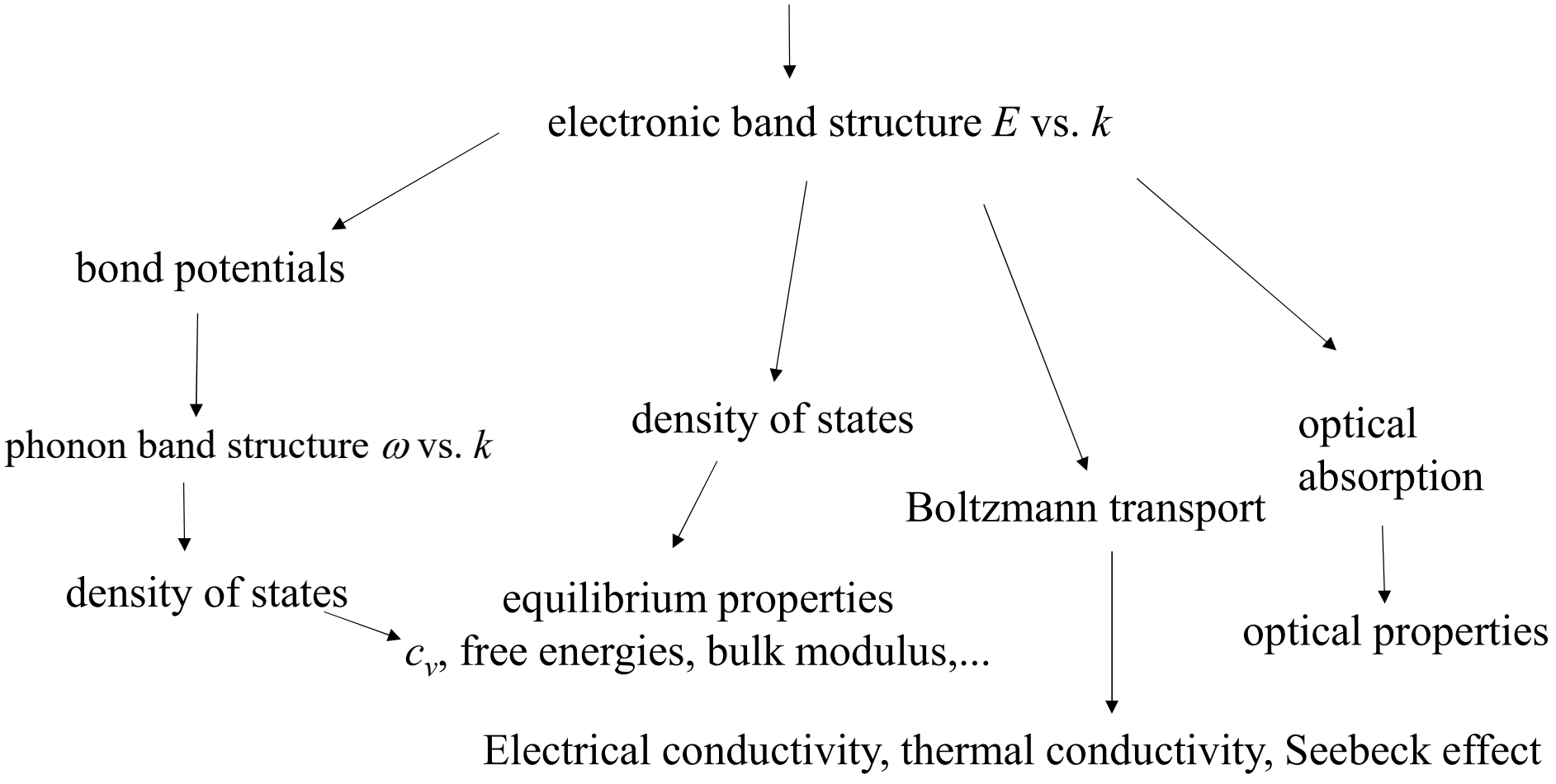
http://lampz.tugraz.at/~hadley/ss1/bands/tbtable/cnt_files/cnts.html

laser-induced pyrolysis of polymers



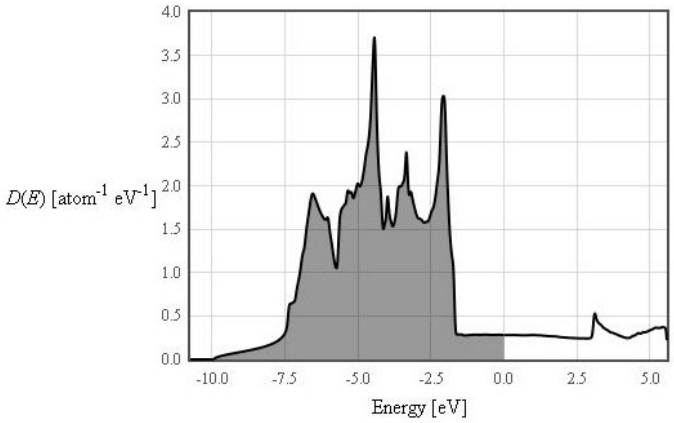
The properties of solids

$$H = -\sum_i \frac{\hbar^2}{2m_e}\nabla_i^2 - \sum_A \frac{\hbar^2}{2m_A}\nabla_A^2 - \sum_{i,A} \frac{Z_A e^2}{4\pi\varepsilon_0 r_{iA}} + \sum_{i<j} \frac{e^2}{4\pi\varepsilon_0 r_{ij}} + \sum_{A<B} \frac{Z_A Z_B e^2}{4\pi\varepsilon_0 r_{AB}}$$



Calculating energies

Electronic component

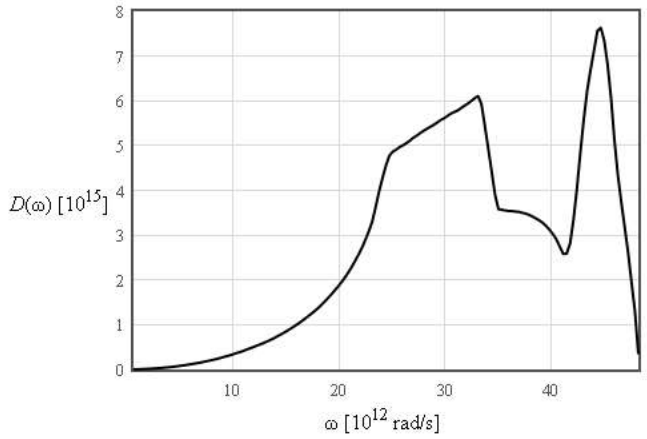


$$n = \int_{-\infty}^{\infty} \frac{D(E)}{1+\exp\left(\frac{E-\mu}{k_B T}\right)} dE$$

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

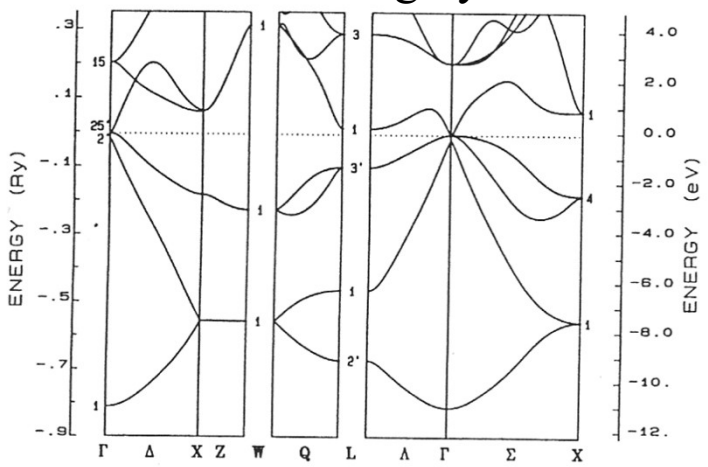
Phonon component

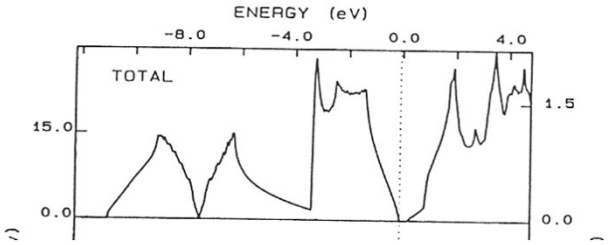
$$u = \int_{-\infty}^{\infty} \frac{ED(E)}{\exp\left(\frac{E-\mu}{k_B T}\right)-1} dE$$

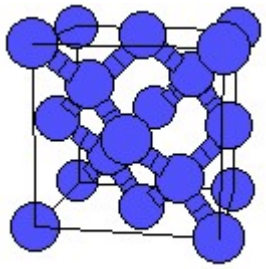


Structural phase transition in Sn

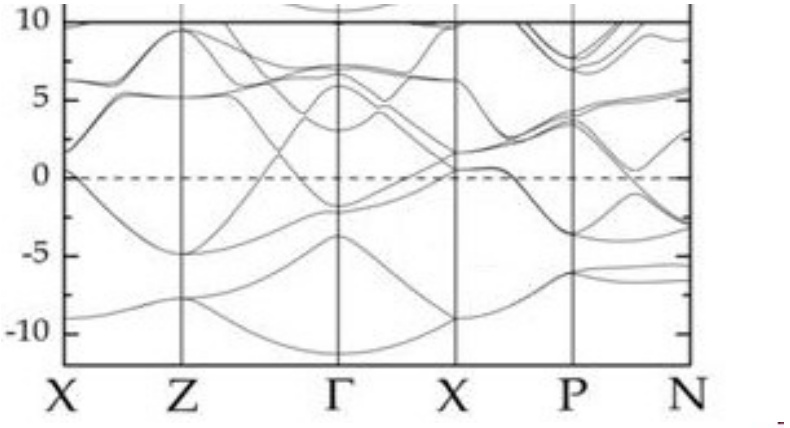
TIN α Sn gray tin

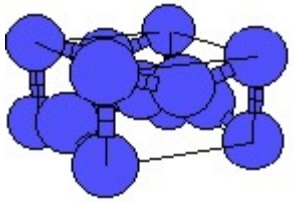






metal β Sn white tin



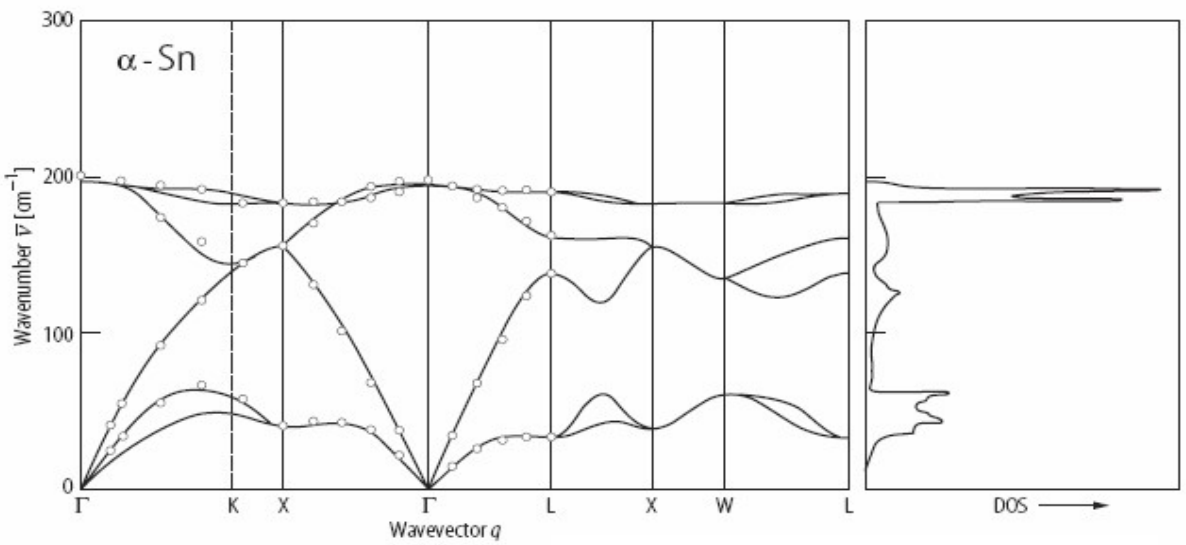


semiconductor: electrons make a negligible contribution to the entropy

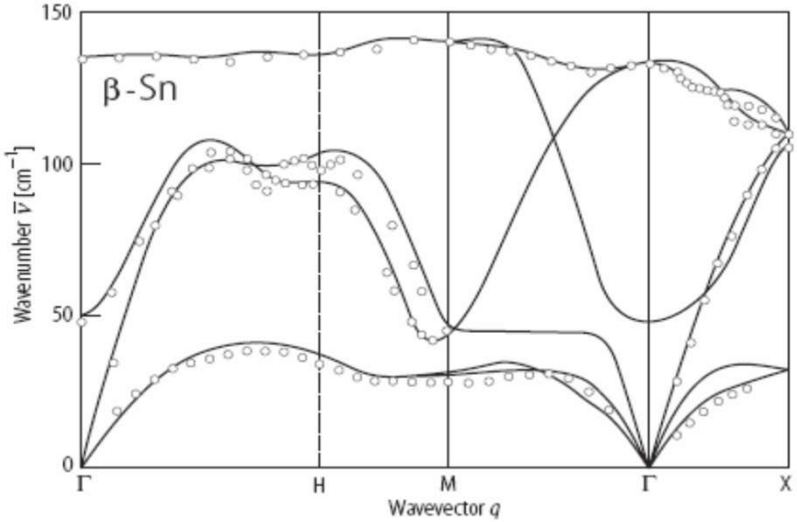
$$s = \frac{\sqrt{2\pi}}{2\pi^2\hbar^3}\left(m_e^* m_h^*\right)^{3/4} \exp\left(\frac{-E_g}{2k_B T}\right)\left(k_B T\right)^{3/2}\left(5k_B + \frac{E_g}{T}\right), \qquad s \approx \frac{\pi^2 D(E_F)}{3} k_B^2 T$$

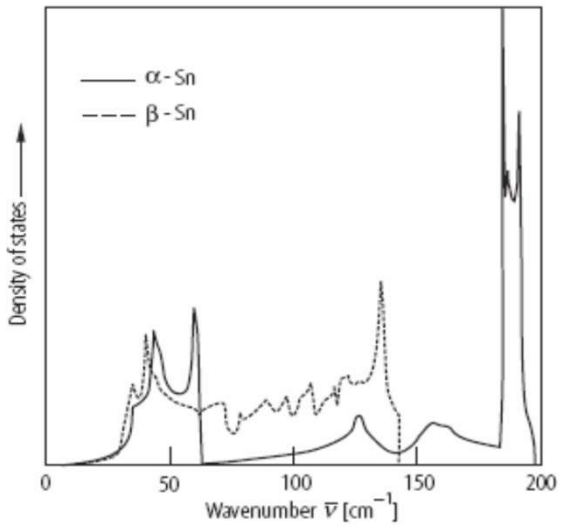
Structural phase transition in Sn

semiconductor
diamond crystal
structure



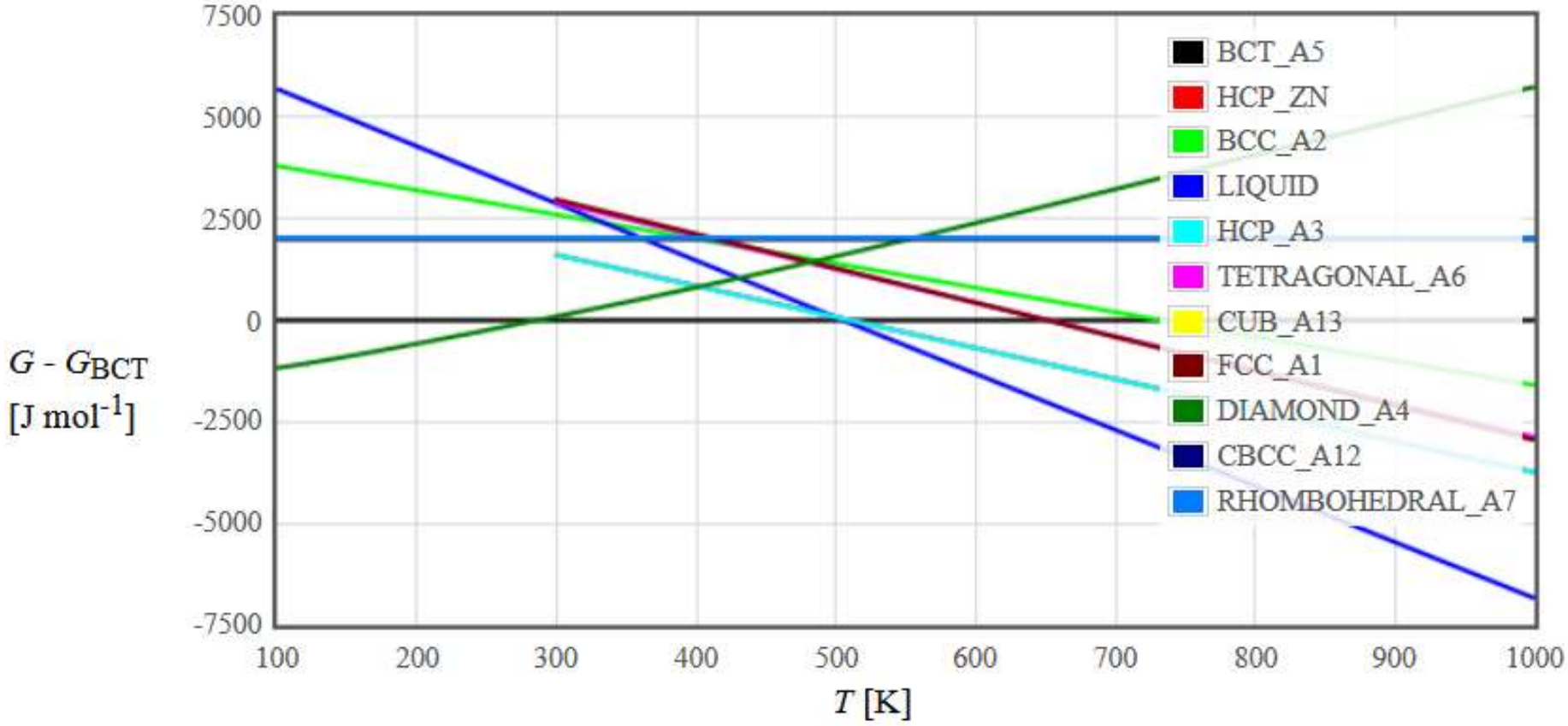
metal
tetragonal
crystal structure





Structural phase transition in Sn

metal β Sn = A5



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