Crystal physics
Semiconductors

rank 2 symmetric tensors[2]	rank 2 asymmetric tensors	rank 3 tensors[3]	rank 4 tensors
$\begin{bmatrix} g_{11} & g_{12} & g_{13} \\ g_{12} & g_{22} & g_{23} \\ g_{13} & g_{23} & g_{33} \end{bmatrix}$	$\begin{bmatrix} g_{11} & g_{12} & g_{13} \\ g_{21} & g_{22} & g_{23} \\ g_{31} & g_{32} & g_{33} \end{bmatrix}$	$\begin{bmatrix} g_{11} & g_{12} & g_{13} & g_{14} & g_{15} & g_{16} \\ g_{21} & g_{22} & g_{23} & g_{24} & g_{25} & g_{26} \\ g_{31} & g_{32} & g_{33} & g_{34} & g_{35} & g_{36} \end{bmatrix}$ reduced, symmetric, asymmetric	$\begin{bmatrix} g_{11} & g_{12} & g_{13} & g_{14} & g_{15} & g_{16} \\ g_{21} & g_{22} & g_{23} & g_{24} & g_{25} & g_{26} \\ g_{31} & g_{32} & g_{33} & g_{34} & g_{35} & g_{36} \\ g_{41} & g_{42} & g_{43} & g_{44} & g_{45} & g_{46} \\ g_{51} & g_{52} & g_{53} & g_{54} & g_{55} & g_{56} \\ g_{61} & g_{62} & g_{63} & g_{64} & g_{65} & g_{66} \end{bmatrix}$ reduced, symmetric, asymmetric
	$\begin{bmatrix} g_{11} & g_{12} & g_{13} \\ g_{21} & g_{22} & g_{23} \\ g_{31} & g_{32} & g_{33} \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$ reduced, symmetric, asymmetric	$\begin{bmatrix} g_{11} & g_{12} & g_{13} & g_{14} & g_{15} & g_{16} \\ g_{21} & g_{22} & g_{23} & g_{24} & g_{25} & g_{26} \\ g_{31} & g_{32} & g_{33} & g_{34} & g_{35} & g_{36} \\ g_{41} & g_{42} & g_{43} & g_{44} & g_{45} & g_{46} \\ g_{51} & g_{52} & g_{53} & g_{54} & g_{55} & g_{56} \\ g_{61} & g_{62} & g_{63} & g_{64} & g_{65} & g_{66} \end{bmatrix}$ reduced, symmetric, asymmetric
$\begin{bmatrix} g_{11} & g_{12} & 0 \\ g_{12} & g_{22} & 0 \\ 0 & 0 & g_{33} \end{bmatrix}$	$\begin{bmatrix} g_{11} & g_{12} & 0 \\ g_{21} & g_{22} & 0 \\ 0 & 0 & g_{33} \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & 0 & g_{14} & g_{15} & 0 \\ 0 & 0 & 0 & g_{24} & g_{25} & 0 \\ g_{31} & g_{32} & g_{33} & 0 & 0 & g_{36} \end{bmatrix}$ reduced, symmetric, asymmetric	$\begin{bmatrix} g_{11} & g_{12} & g_{13} & 0 & 0 & g_{16} \\ g_{21} & g_{22} & g_{23} & 0 & 0 & g_{26} \\ g_{31} & g_{32} & g_{33} & 0 & 0 & g_{36} \\ 0 & 0 & 0 & g_{44} & g_{45} & 0 \\ 0 & 0 & 0 & g_{54} & g_{55} & 0 \\ g_{61} & g_{62} & g_{63} & 0 & 0 & g_{66} \end{bmatrix}$ reduced, symmetric, asymmetric
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http://lamp.tu-graz.ac.at/~hadley/ss2/crystalphysics/crystalclasses/crystalclasses.html

Electrostriction

$$\frac{\partial P_k}{\partial \sigma_{ij}} = \frac{\partial \varepsilon_{ij}}{\partial E_k} = -\left(\frac{\partial^2 G}{\partial E_k \partial \sigma_{ij}} \right) = d_{ijk}$$

$$\epsilon_{ij} = d_{ijk} E_k + Q_{ijkl} E_k E_l + \cdots$$

piezoelectricity

Electrostriction

Nonlinear optics

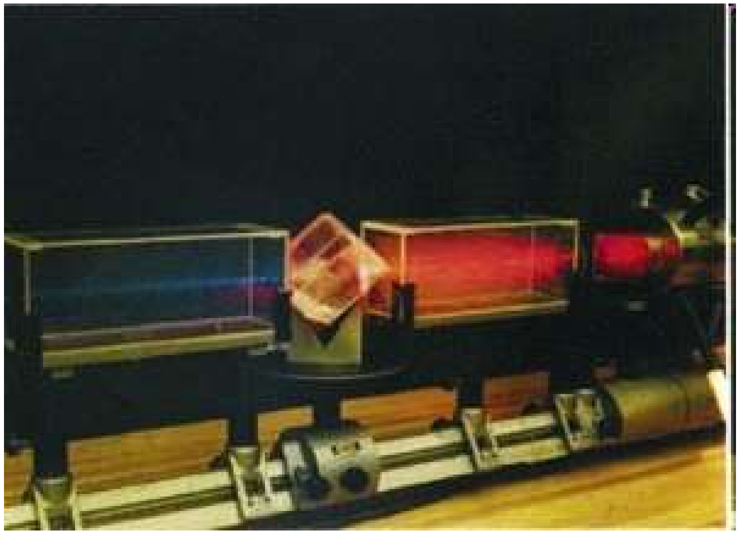
Period doubling crystals

no inversion symmetry

$$P = \chi^{(1)}E + \chi^{(2)}E^2 + \chi^{(3)}E^3 + \cdots$$

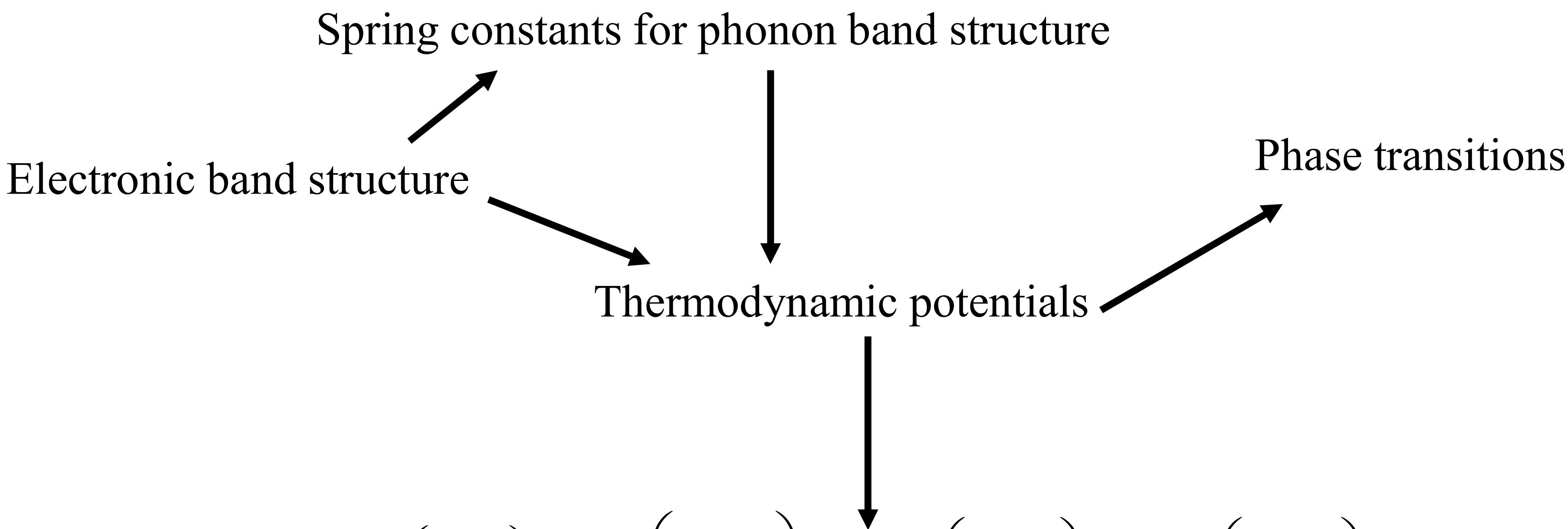
$$P_i = \frac{-\partial^2 G}{\partial E_i \partial E_j} E_j + \frac{1}{2}\frac{-\partial^3 G}{\partial E_i \partial E_j \partial E_k} E_j E_k + \cdots$$

$$\cos^2(\omega t) = \tfrac{1}{2}\left(1 + \cos(2\omega t)\right)$$



806 nm light : lithium iodate ($LiIO_3$)
860 nm light : potassium niobate ($KNbO_3$)
980 nm light : $KNbO_3$
1064 nm light : monopotassium phosphate (KH_2PO_4, KDP), lithium triborate (LBO).
1300 nm light : gallium selenide (GaSe)
1319 nm light : $KNbO_3$, BBO, KDP, lithium niobate ($LiNbO_3$), $LiIO_3$

Thermodynamic properties



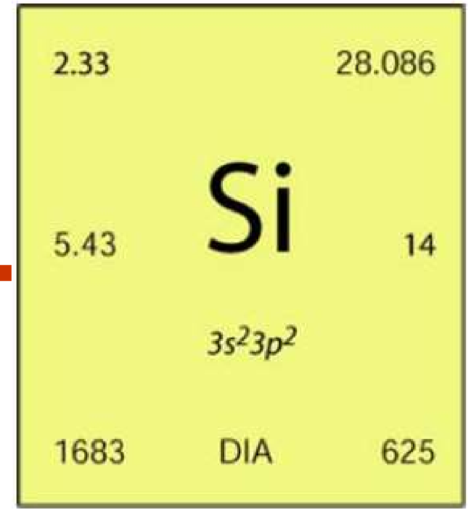
total derivative: $$dG = \left(\frac{\partial G}{\partial T}\right) dT + \left(\frac{\partial G}{\partial \sigma_{ij}}\right) d\sigma_{ij} + \left(\frac{\partial G}{\partial E_k}\right) dE_k + \left(\frac{\partial G}{\partial H_l}\right) dH_l$$

$$\left(\frac{\partial G}{\partial \sigma_{ij}}\right) = -\varepsilon_{ij} \qquad \left(\frac{\partial G}{\partial E_k}\right) = -P_k$$

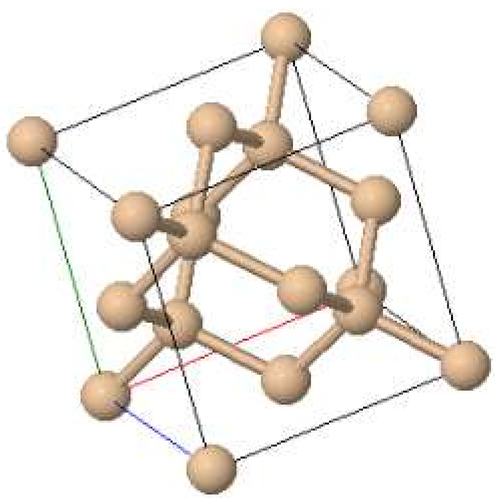
$$\left(\frac{\partial G}{\partial H_l}\right) = -M_l \qquad \left(\frac{\partial G}{\partial T}\right) = -S$$

Semiconductors

Silicon

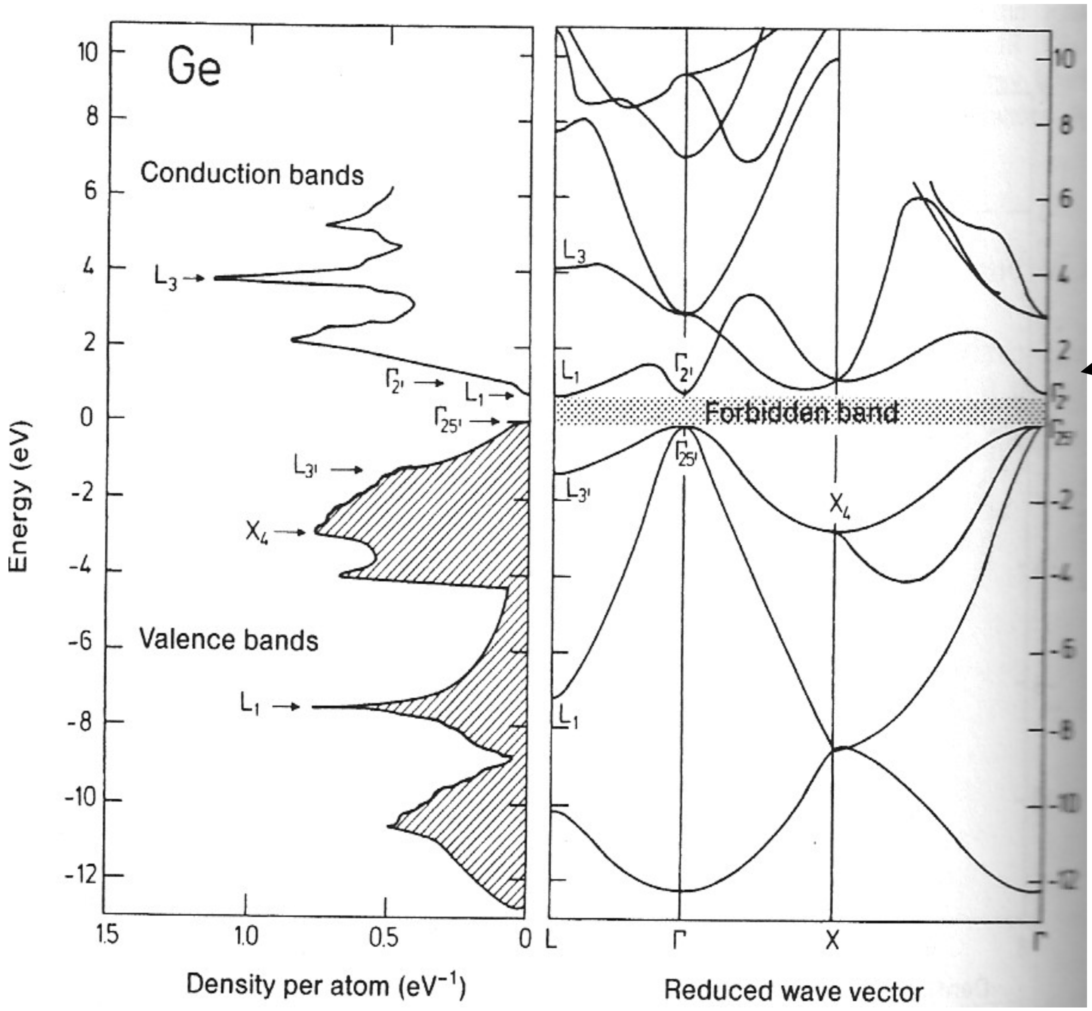


- Important semiconducting material
- 2nd most common element on earths crust (rocks, sand, glass, concrete)
- Often doped with other elements
- Oxide SiO_2 is a good insulator



silicon crystal = diamond crystal structure

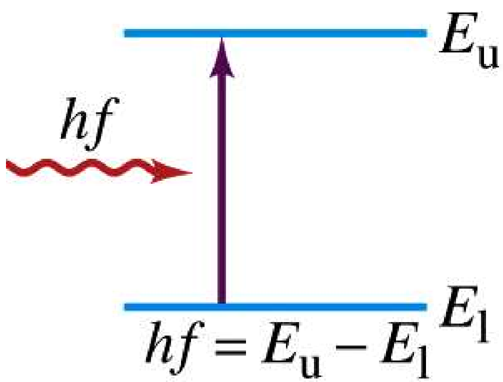
Semiconductors



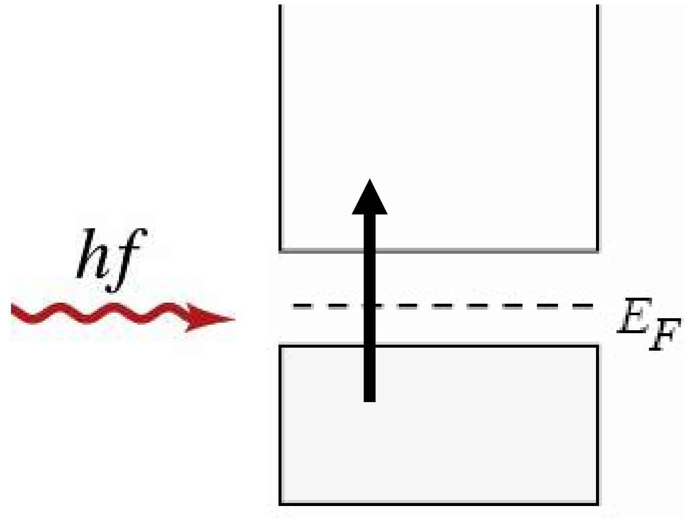
$$n = \int_{-\infty}^{\infty} D(E) f(E) dE$$

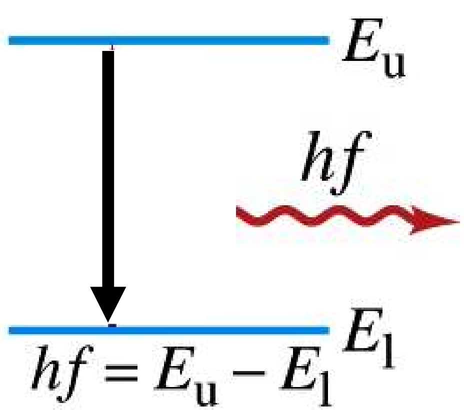
From Ibach & Lueth

Absorption and emission of photons

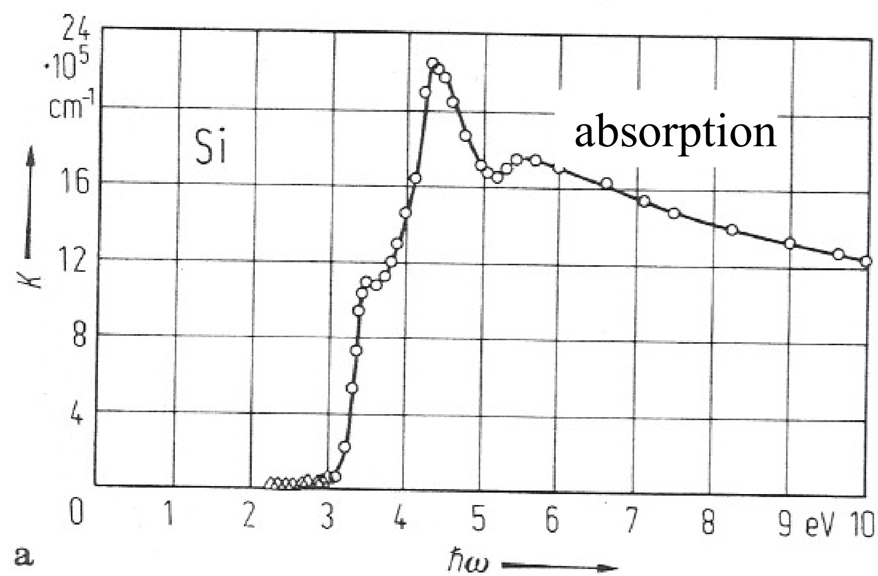


absorption

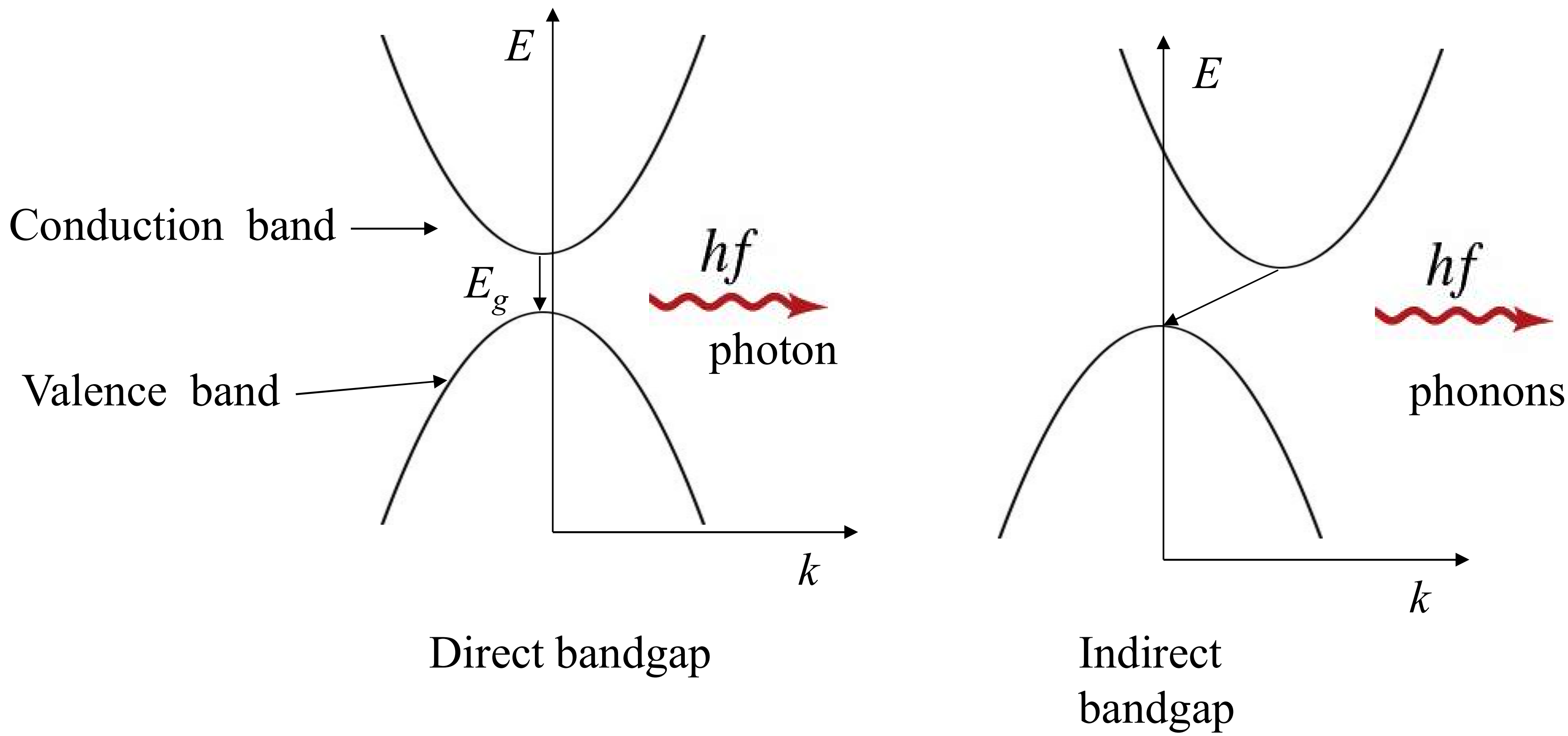




emission

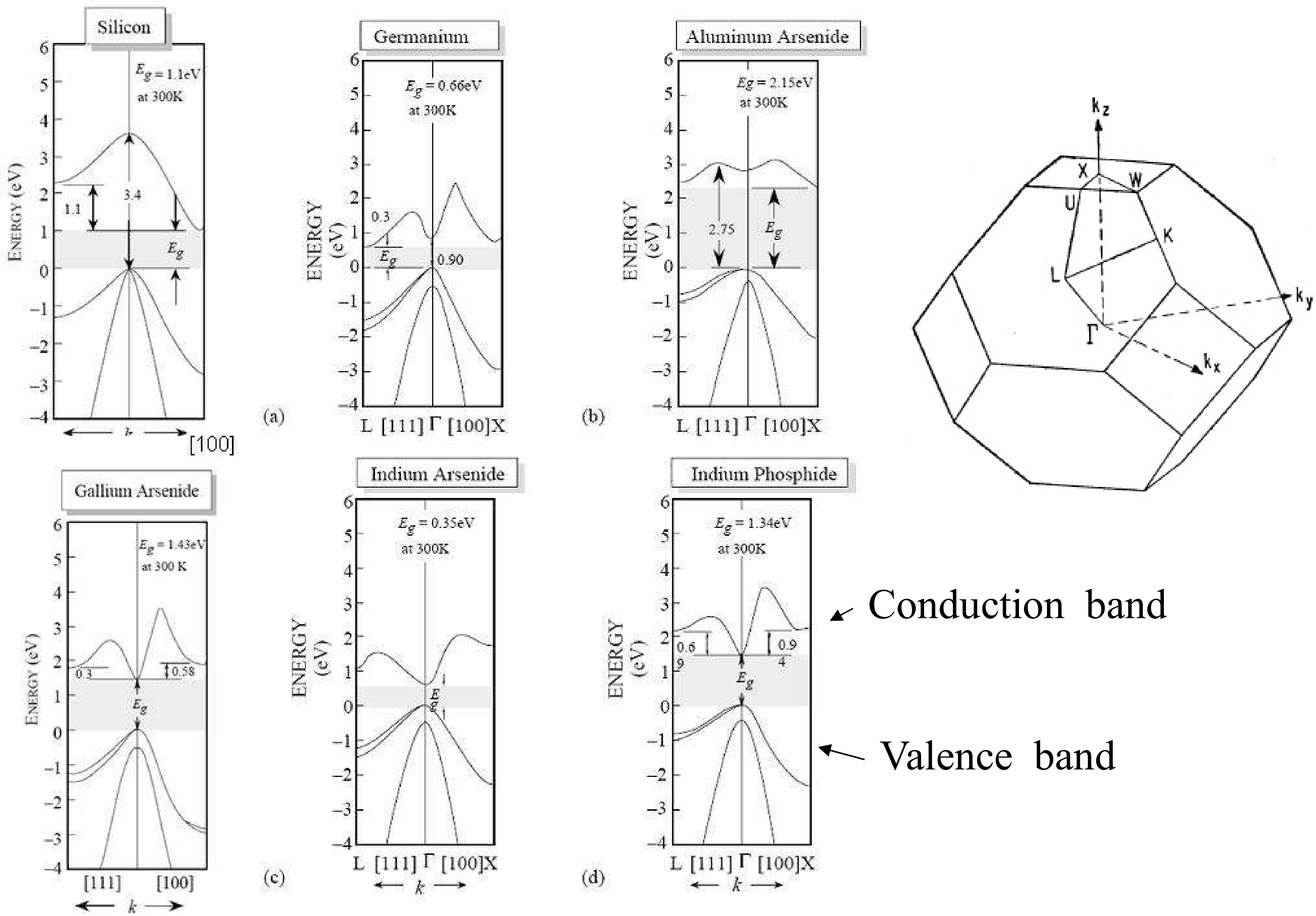


Direct and indirect band gaps



Direct bandgap semiconductors are used for optoelectronics

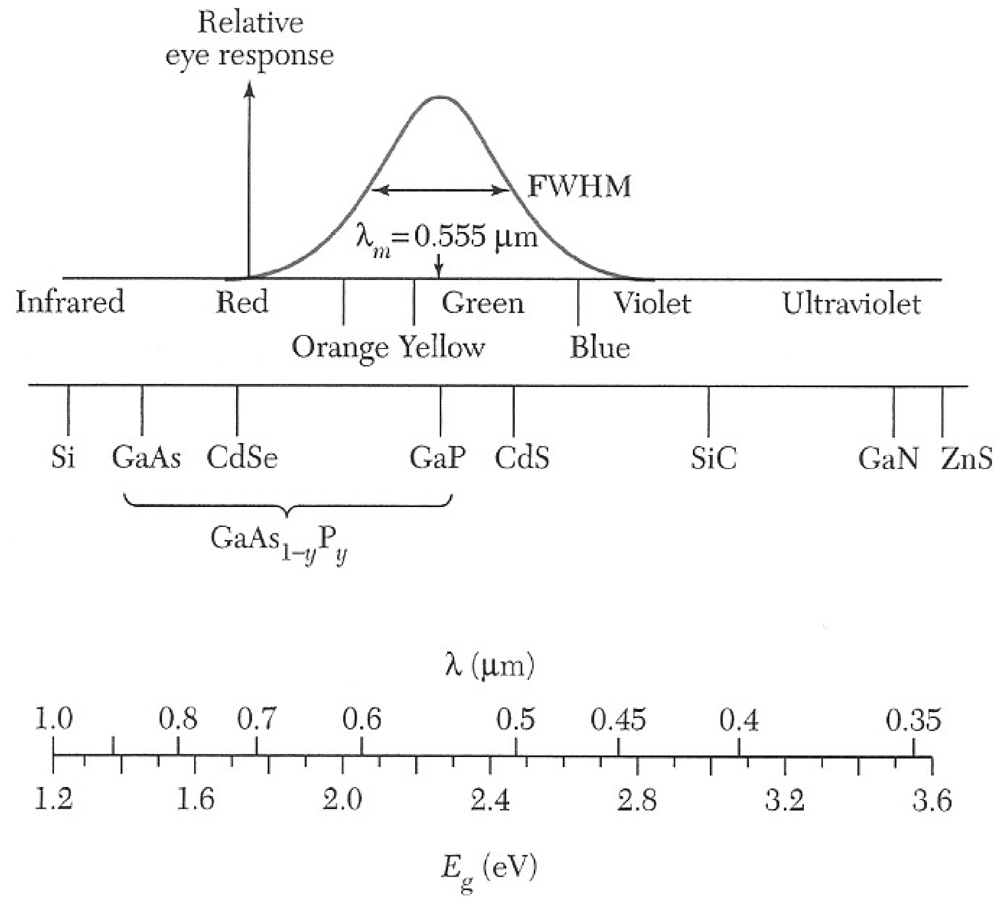
Semiconductors



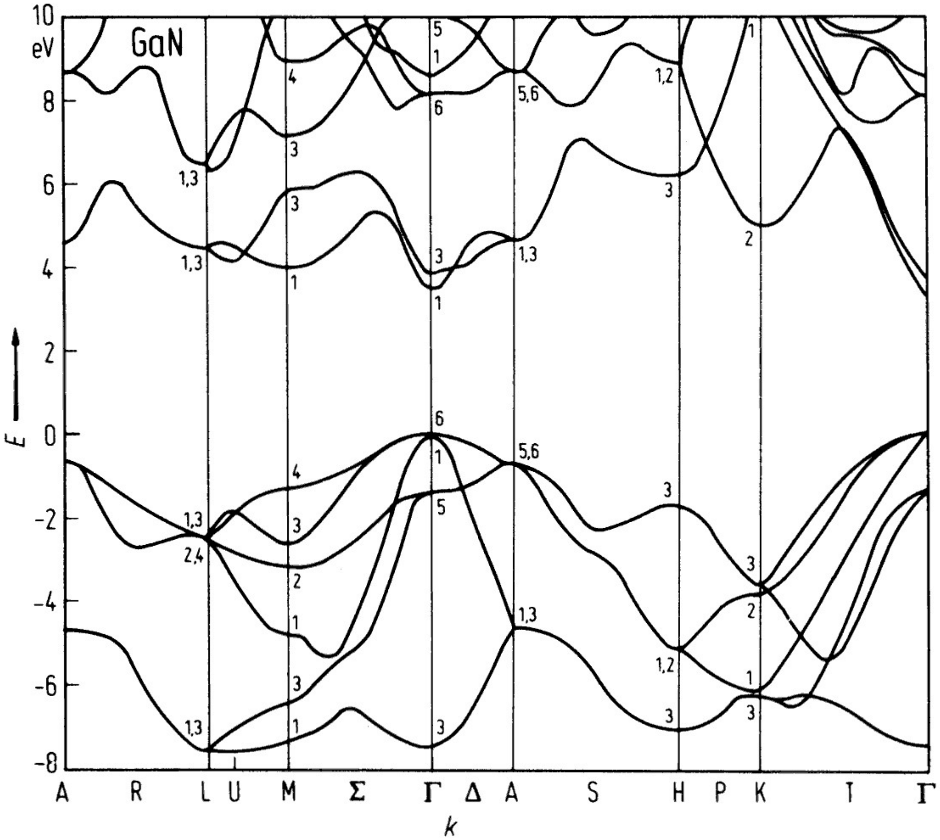
Light emitting diodes

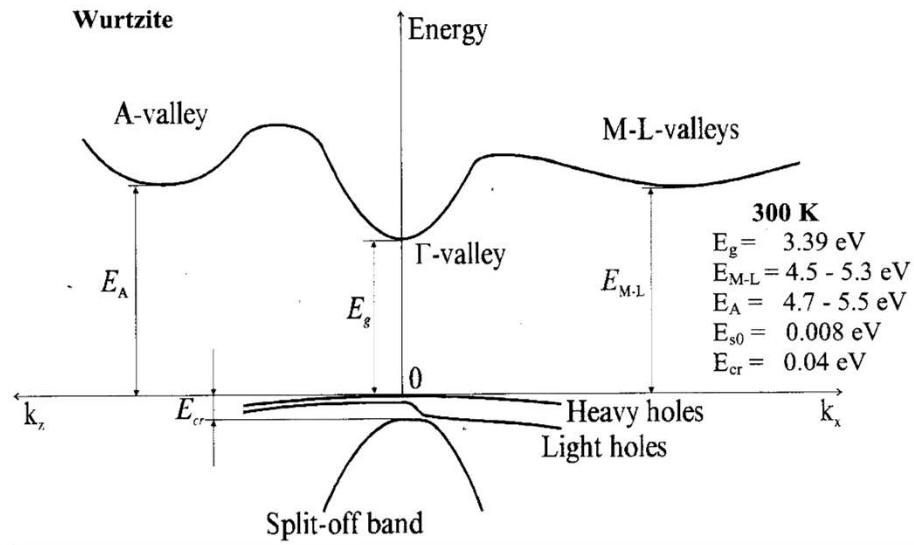
TABLE 1 Common III-V materials used to produce LEDs and their emission wavelengths.

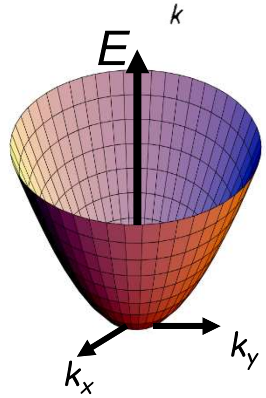
Material	Wavelength (nm)
InAsSbP/InAs	4200
InAs	3800
GaInAsP/GaSb	2000
GaSb	1800
$Ga_xIn_{1-x}As_{1-y}P_y$	1100-1600
$Ga_{0.47}In_{0.53}As$	1550
$Ga_{0.27}In_{0.73}As_{0.63}P_{0.37}$	1300
GaAs:Er,InP:Er	1540
Si:C	1300
GaAs:Yb,InP:Yb	1000
$Al_xGa_{1-x}As$:Si	650-940
GaAs:Si	940
$Al_{0.11}Ga_{0.89}As$:Si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

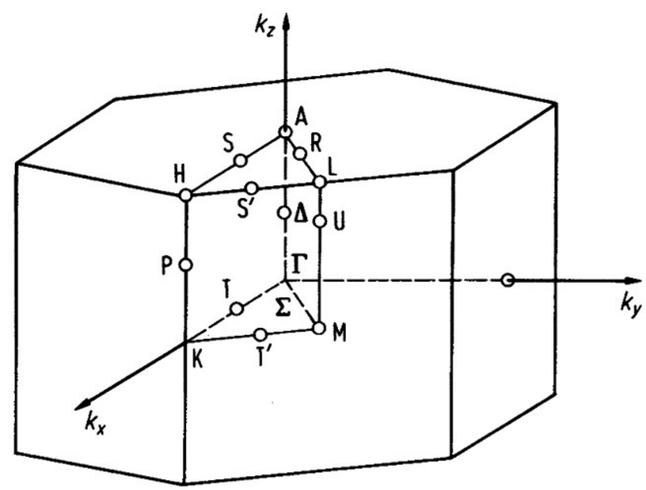


GaN





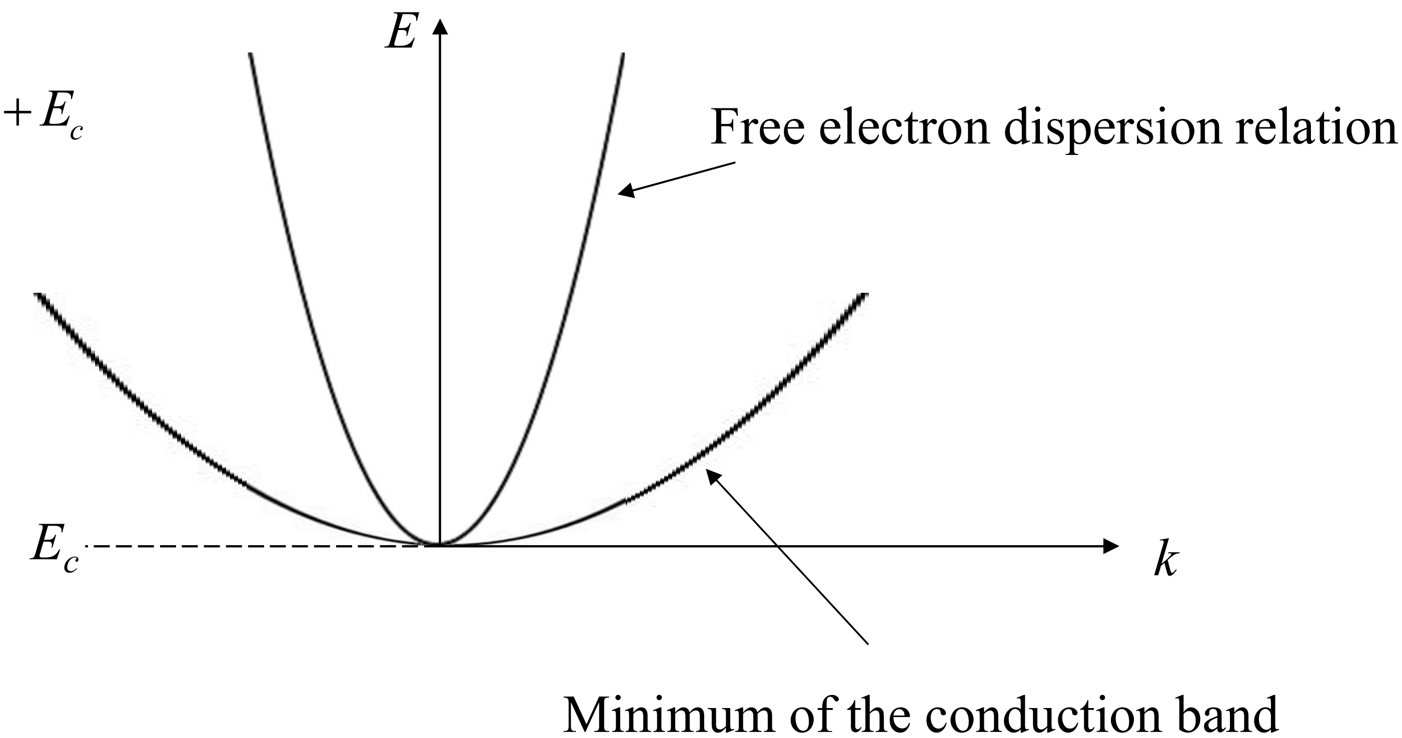




1st Brillioun zone of hcp

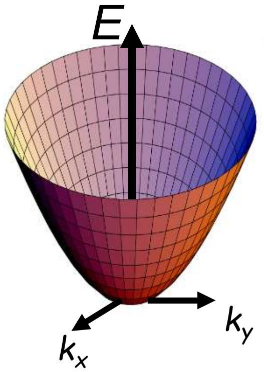
Conduction band minimum

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



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

Effective mass



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

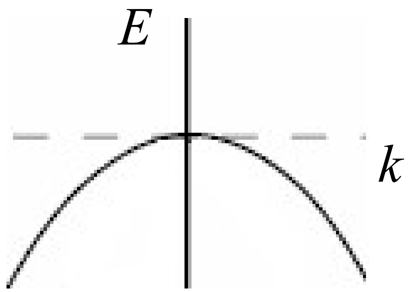
The parabola at the bottom of the conduction band does not have the same curvature as the free-electron dispersion relation. We define an effective mass to characterize the conduction band minimum.

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

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 = effective mass of holes

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

Holes

A completely filled band does not contribute to the current.

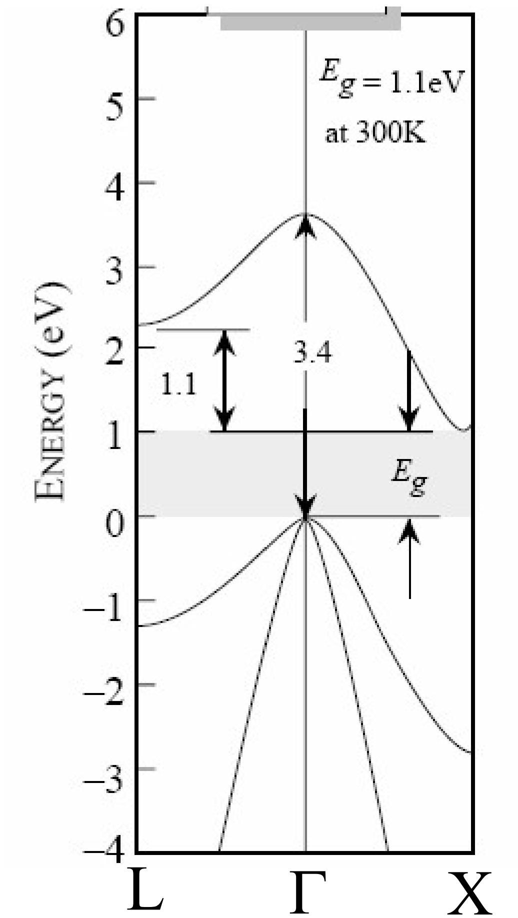
$$\vec{j} = \int_{\text{filled states}} -e\vec{v}(\vec{k})D(\vec{k})f(\vec{k})d\vec{k}$$

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

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

Holes have a positive charge and a positive mass.

Effective Mass



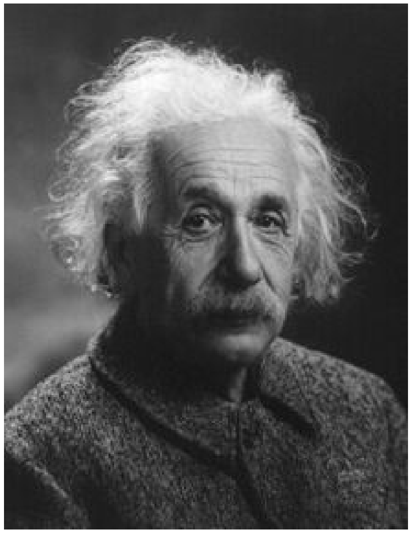
$$E = \frac{\hbar^2\left(\vec{k}-\vec{k}_0\right)^2}{2m^*} + E_c$$

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

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

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

Holes

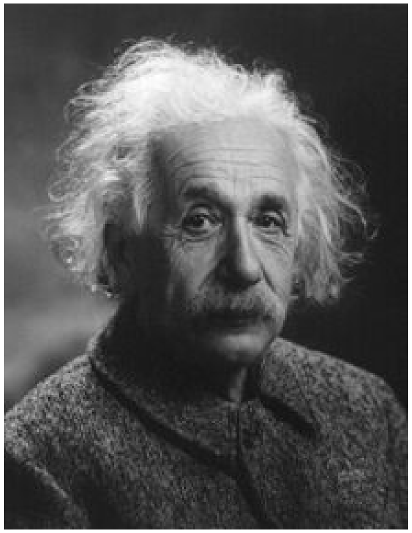


Albert Einstein

Erwin Schrödinger

Paul Adrien Maurice Dirac

Holes



Albert Einstein

Erwin Schrödinger

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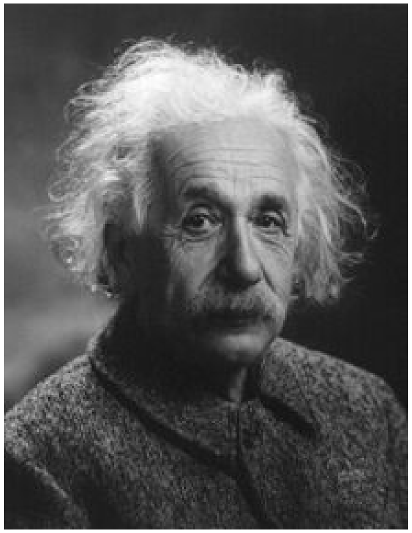
$$\frac{d^2u}{dt^2} = c^2 \frac{d^2u}{dx^2}$$

Wave equation

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

Heat equation

Holes



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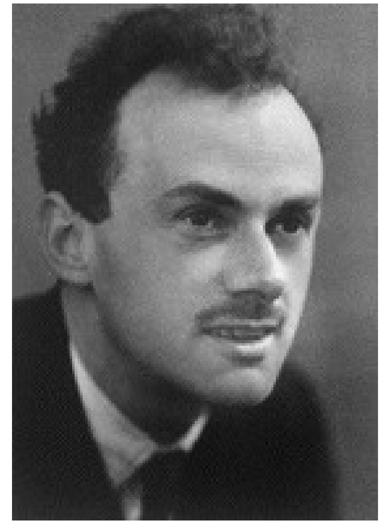

Paul Adrien Maurice Dirac

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

Dirac equation