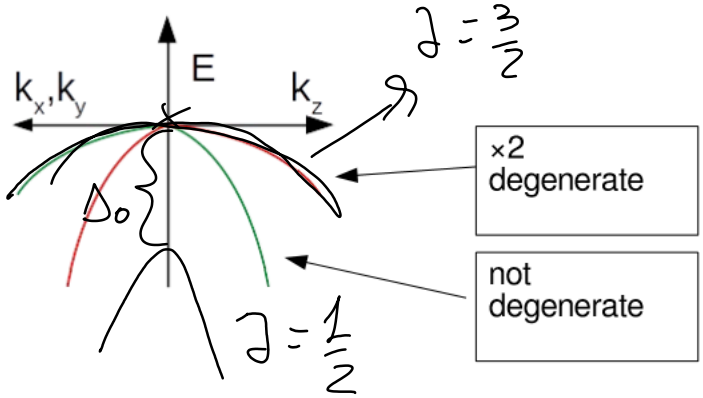
Spin-orbit interaction in the valence band

- **Valence band and spin-orbit interaction**
- **Total angular momentum of valence band states**
- **Heavy-hole, light-hole and split-off states**

Spin orbit interaction



Starting from the three p_x, p_y and p_z orbitals three bands are formed

Since p states have an orbital angular momentum **L** ≠0. Spin-orbit interaction needs to be considered

$$H_{so} = \lambda \boldsymbol{L} \cdot \boldsymbol{S}$$

$$< \mathbf{L} \cdot \mathbf{S} > = \frac{1}{2} < \mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2 >$$

$$\frac{}{\hbar^2}$$

$$= \frac{\lambda}{2}\left(j(j+1) - l(l+1) - s(s+1)\right)$$

$H_{so} = \lambda (\vec{L} \cdot \vec{S})$ $\quad \vec{J} = \vec{L} + \vec{S}$

$\lambda \propto Z^4$ $\quad \vec{J} \cdot \vec{J} = J^2 = (\vec{L} + \vec{S}) \cdot (\vec{L} + \vec{S})$

$= L^2 + S^2 + 2\vec{L} \cdot \vec{S}$

$\vec{L} \cdot \vec{S} = \frac{1}{2}(J^2 - L^2 - S^2)$

$L^2 = \hbar^2(l(l+1))$ $\quad S^2 = \hbar^2(s(s+1))$

$P \rightarrow l = 1$

$S \rightarrow l = \emptyset$

$J^2 = \hbar^2(j(j+1))$

$l + s = \frac{3}{2}$ $\quad j = \frac{3}{2}$ $\quad j_z = +\frac{3}{2}, +\frac{1}{2}, -\frac{1}{2}, -\frac{3}{2}$

j

$l - s = \frac{1}{2}$ $\quad j = \frac{1}{2}$ $\quad j_z = +\frac{1}{2}, -\frac{1}{2}$

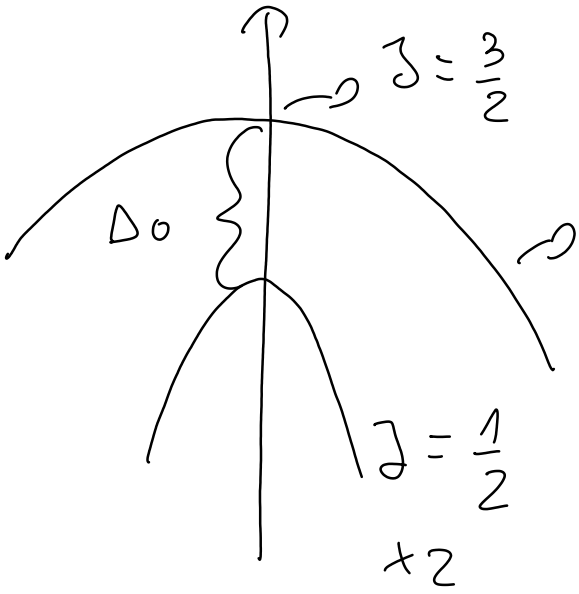
$H_{so} = \frac{\lambda}{2}(J^2 - L^2 - S^2)$

$l = 1$ $\quad s = \frac{1}{2}$

$$H_{so} = \frac{1}{2} q^2 \left(\hat{J}(\hat{J}+1) - \hat{l}(\hat{l}+1) - \hat{S}(\hat{S}+1) \right)$$

$$J = \frac{3}{2} \quad , \quad J = \frac{1}{2}$$

$$\Delta_0 = H_{so}\left(J=\tfrac{3}{2}\right) - H_{so}\left(J=\tfrac{1}{2}\right) = \frac{3}{2} \Lambda^4$$



$J_z = +\frac{3}{2} \; +\frac{1}{2} \; -\frac{1}{2} \; -\frac{3}{2}$

$J_z = +\frac{1}{2} \; +\frac{1}{2}$

$P_x |\uparrow\rangle \rightarrow J, J_z$

$|1/2, 1\rangle$

$$P_x = \frac{1}{\sqrt{2}} \left(-|1/2, 1\rangle + |1, -1\rangle \right) |\uparrow\rangle$$

CLEBSCH-GORDAN COEFF.

ϕ

J, J_z

$$\phi_{\frac{3}{2},+\frac{3}{2}} = -\frac{1}{\sqrt{2}}(P_x + iP_y)\uparrow \qquad \phi_{\frac{3}{2},-\frac{3}{2}}$$

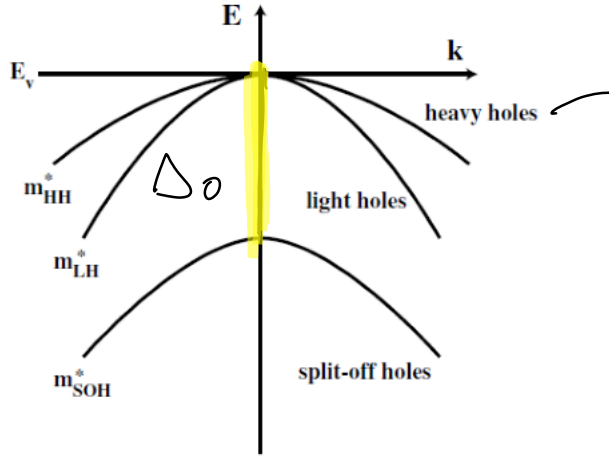
$$\phi_{\frac{3}{2},+\frac{1}{2}} = -\frac{1}{\sqrt{6}}\left((P_x + iP_y)\downarrow - 2P_z\uparrow\right) \qquad \phi_{\frac{3}{2},-}$$

$$\phi_{\frac{1}{2},+\frac{1}{2}} = -\frac{1}{\sqrt{3}}\left[(P_x + iP_y)\downarrow + P_z\uparrow\right] \qquad \phi_{\frac{1}{2},}$$

Valence band structure

Spin-orbit removes the degeneracy of the two upper bands. The different bands can be labelled according to the two quantum numbers: J (total angular momentum) and J_z (projection of the total angular momentum). Considering that for p states $l=1$ and $s=1/2$, the VB states will have $J=3/2$ or $J=1/2$. $J=3/2$ states lay higher in energy and will be separated by a spin-orbit energy Δ from the 'split-off' (SO) states with $J=1/2$. The $J=3/2$ states can be further divided according to the quantum number J_z. We will therefore have $J_z = \pm 3/2$ or $J_z = \pm 1/2$.

Effective mass	J	J_z
HH	3/2	±3/2
LH	3/2	±1/2
SO	1/2	±1/2



Valence band structure

The eigenvector are obtained from the Clebsch-Gordan coefficients. They feature well defined values of: j, j_z l and s (not m and s_z)

Heavy holes

$$\Phi_{3/2,3/2} = \phi_{1,1}\uparrow = \frac{-1}{\sqrt{2}}(p_x + ip_y)\uparrow$$

$$\Phi_{3/2,-3/2} = \phi_{1,-1}\downarrow = \frac{1}{\sqrt{2}}(p_x - ip_y)\downarrow$$

Light holes

$$\Phi_{3/2,1/2} = \frac{1}{\sqrt{3}}\phi_{1,1}\downarrow + \frac{\sqrt{2}}{\sqrt{3}}\phi_{1,0}\uparrow = \frac{-1}{\sqrt{6}}[(p_x + ip_y)\downarrow - 2p_z\uparrow]$$

$$\Phi_{3/2,-1/2} = \frac{\sqrt{2}}{\sqrt{3}}\phi_{1,0}\downarrow + \frac{1}{\sqrt{3}}\phi_{1,-1}\uparrow = \frac{1}{\sqrt{6}}[(p_x - ip_y)\uparrow + 2p_z\downarrow]$$

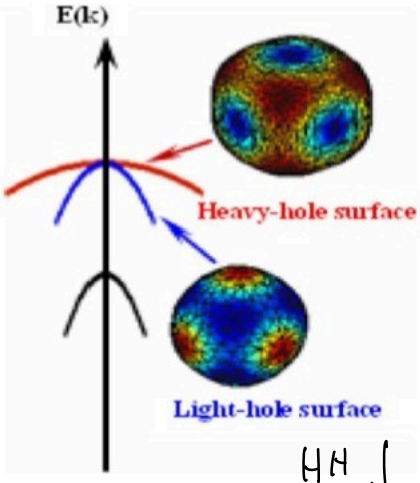
Split-off

$$\Phi_{1/2,1/2} = \frac{-1}{\sqrt{3}}\phi_{1,0}\uparrow + \frac{\sqrt{2}}{\sqrt{3}}\phi_{1,1}\downarrow = \frac{-1}{\sqrt{3}}[(p_x + ip_y)\downarrow + p_z\uparrow]$$

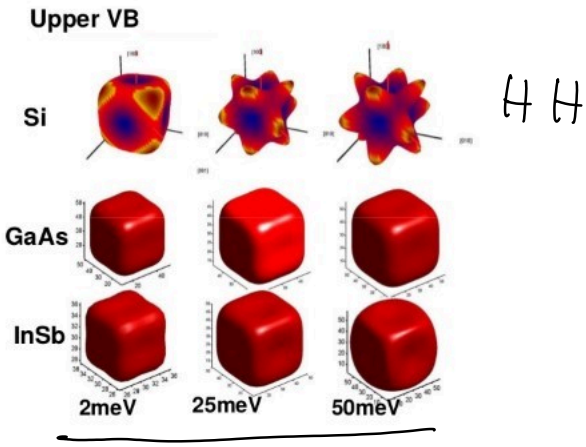
$$\Phi_{1/2,-1/2} = \frac{-\sqrt{2}}{\sqrt{3}}\phi_{1,-1}\uparrow + \frac{1}{\sqrt{3}}\phi_{1,0}\downarrow = \frac{-1}{\sqrt{3}}[(p_x - ip_y)\uparrow - p_z\downarrow]$$

Valence band structure

Isoenergy surfaces



HH



HH

Figure 2 : Isoenergy surfaces for upper valence band in silicon, GaAs and InSb at 2meV / 25 meV / 50 meV.

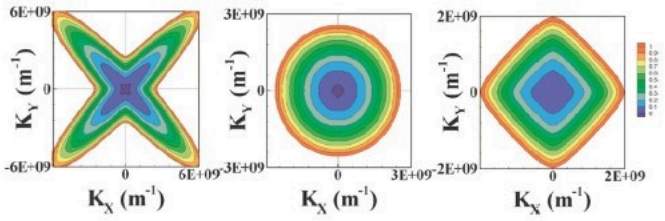
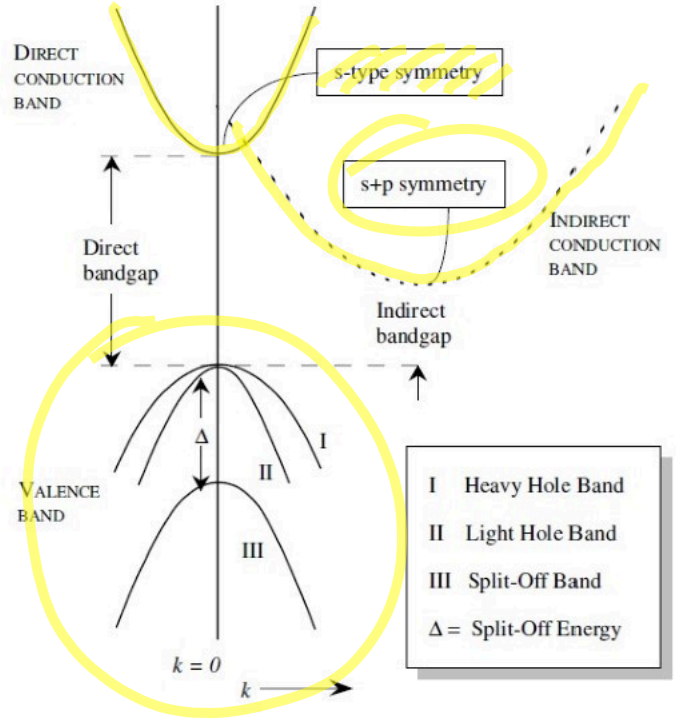


Figure 5. 3D equienergy surfaces of heavy hole, light hole and split off band in Si for $k_z = 0$.

Valence band structure

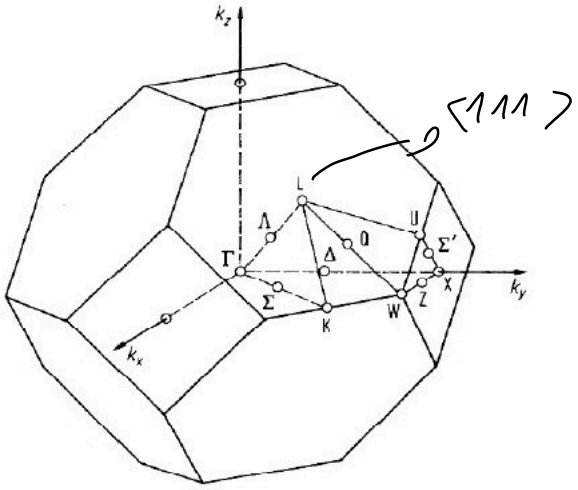


SPHERICAL HARMONIC

$$
\begin{aligned}
\text{HH} \quad \Phi_{3/2,3/2} &= \phi_{1,1}\uparrow \\
&= \frac{-1}{\sqrt{2}}(p_x + ip_y)\uparrow \\
\text{LH} \quad \Phi_{3/2,1/2} &= \frac{1}{\sqrt{3}}\phi_{1,1}\downarrow + \frac{\sqrt{2}}{\sqrt{3}}\phi_{1,0}\uparrow \\
&= \frac{-1}{\sqrt{6}}\left[(p_x + ip_y)\downarrow - 2p_z\uparrow\right] \\
\text{LH} \quad \Phi_{3/2,-1/2} &= \frac{\sqrt{2}}{\sqrt{3}}\phi_{1,0}\downarrow + \frac{1}{\sqrt{3}}\phi_{1,-1}\uparrow \\
&= \frac{1}{\sqrt{6}}\left[(p_x - ip_y)\uparrow + 2p_z\downarrow\right] \\
\text{HH} \quad \Phi_{3/2,-3/2} &= \phi_{1,-1}\downarrow \\
&= \frac{1}{\sqrt{2}}(p_x - ip_y)\downarrow \\
\text{SO} \quad \Phi_{1/2,1/2} &= \frac{-1}{\sqrt{3}}\phi_{1,0}\uparrow + \frac{\sqrt{2}}{\sqrt{3}}\phi_{1,1}\downarrow \\
&= \frac{-1}{\sqrt{3}}\left[(p_x + ip_y)\downarrow + p_z\uparrow\right] \\
\text{SO} \quad \Phi_{1/2,-1/2} &= \frac{-\sqrt{2}}{\sqrt{3}}\phi_{1,-1}\uparrow + \frac{1}{\sqrt{3}}\phi_{1,0}\downarrow \\
&= \frac{-1}{\sqrt{3}}\left[(p_x - ip_y)\uparrow - p_z\downarrow\right]
\end{aligned}
$$

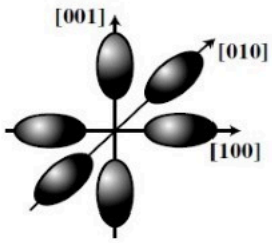
High symmetry points in semiconductors

The Brillouin zone (BZ) of an FCC lattice
Γ is the center of the BZ ($k=0$)
Δ (delta) is the <100> directions (e.g. $k_x \neq 0$, $k_y = k_z = 0$) connecting Γ to X
Λ (lambda) is the <111> directions ($k_x = k_y = k_z \neq 0$) connecting Γ to L
Σ (sigma) is the <110> directions connecting Γ to K

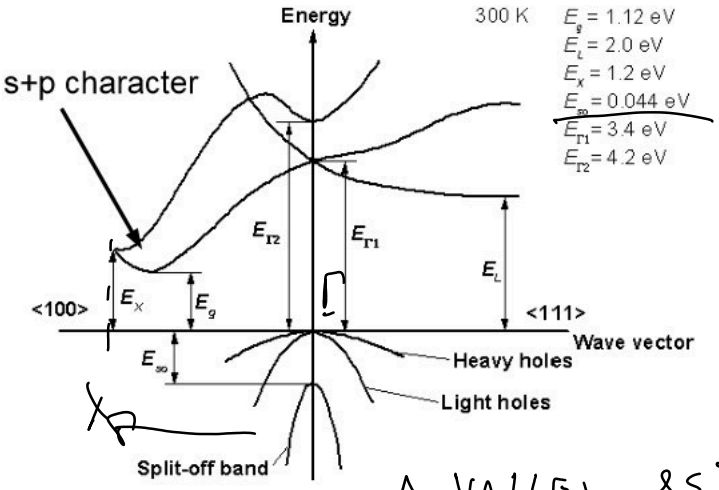


Silicon

Silicon is an indirect semiconductor.
The CB minima is at 85% of the 1st BZ along Δ.
In Si there are 6 'Δ minima' or 'Δ valleys'.



Position of the CB minima in reciprocal space

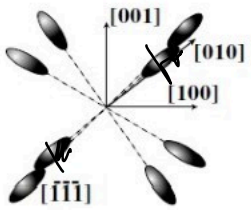


Δ-VALLEY 85% Δ

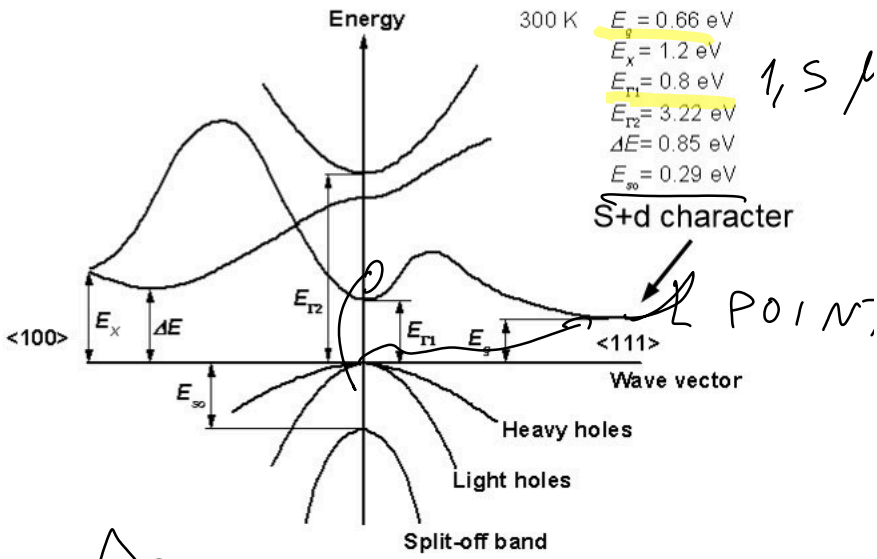
$\Delta_0 = 40$ meV

Germanium

Germanium is an indirect semiconductor.
The CB minima is at L
In Ge there are 4 'L minima' or 'L valleys'.



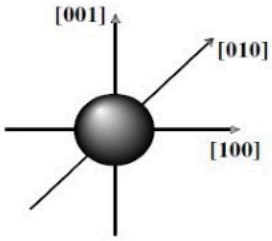
Position of the CB minima in reciprocal space



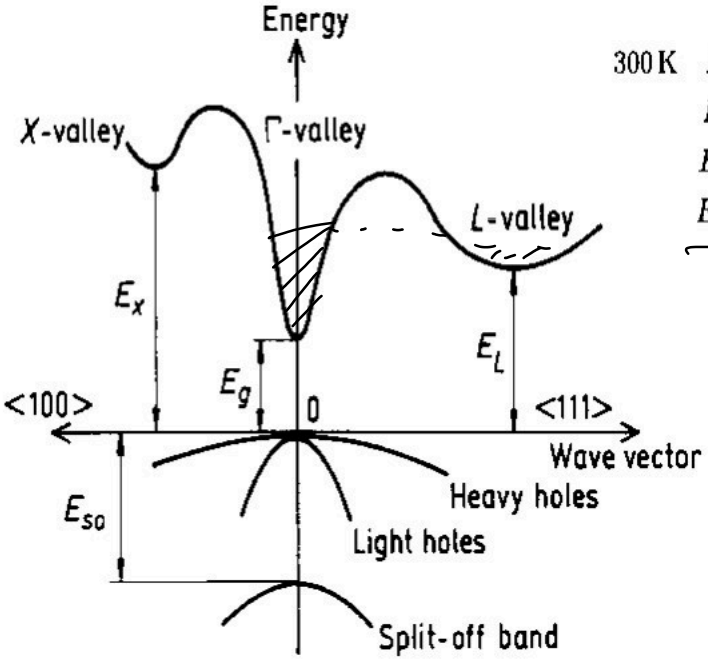
Δ_0

GaAs

Gallium arsenide is a direct semiconductor.
The CB minima is at Γ
In GaAs there is one 'Γ minimum'.



Position of the CB minima in reciprocal space

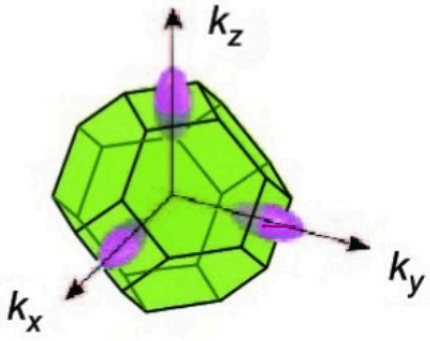


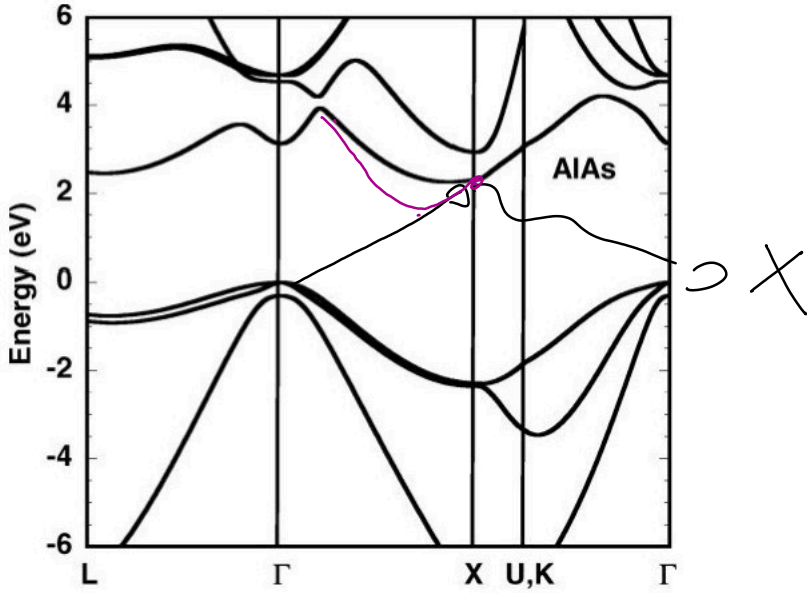
300 K $E_g = 1.42$ eV
$E_L = 1.71$ eV
$E_X = 1.90$ eV
$E_{so} = 0.34$ eV

AlAs

Aluminum arsenide is an indirect gap semiconductor
The CB minima is at X
In AlAs there are 3 X minima

Eg= 2.239 eV





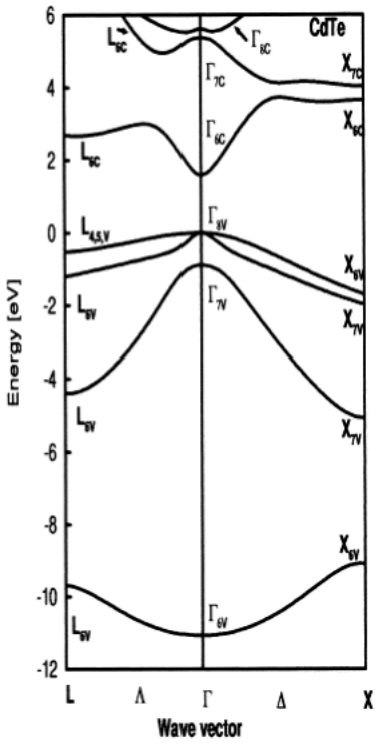
3 X

CdTe

Cadmium telluride is a direct gap semiconductor

Eg=1.5 eV

Used for solar cells, and IR windows



GaN

Gallium nitride is a direct semiconductor.
The CB minima is at Γ