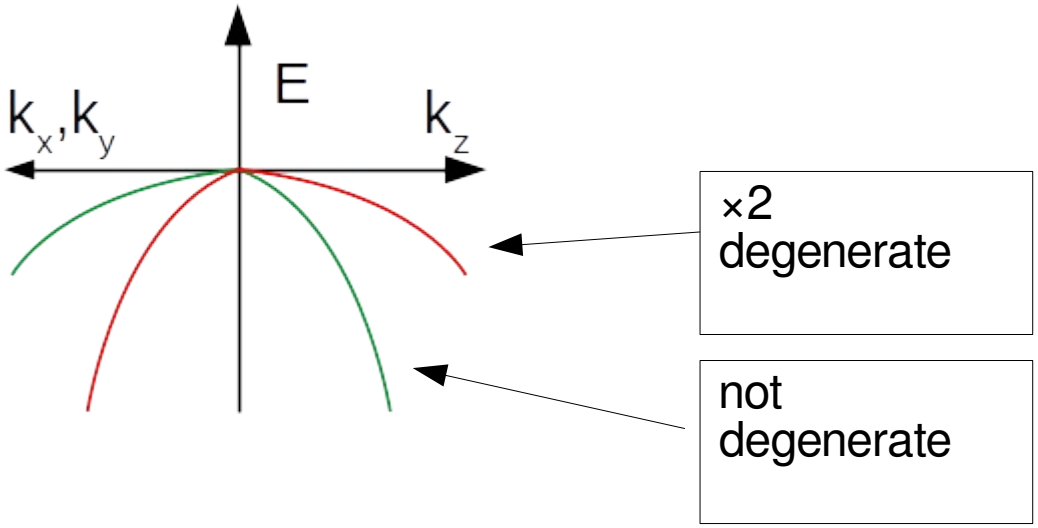
Spin-orbit interaction in the valence band

- **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

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

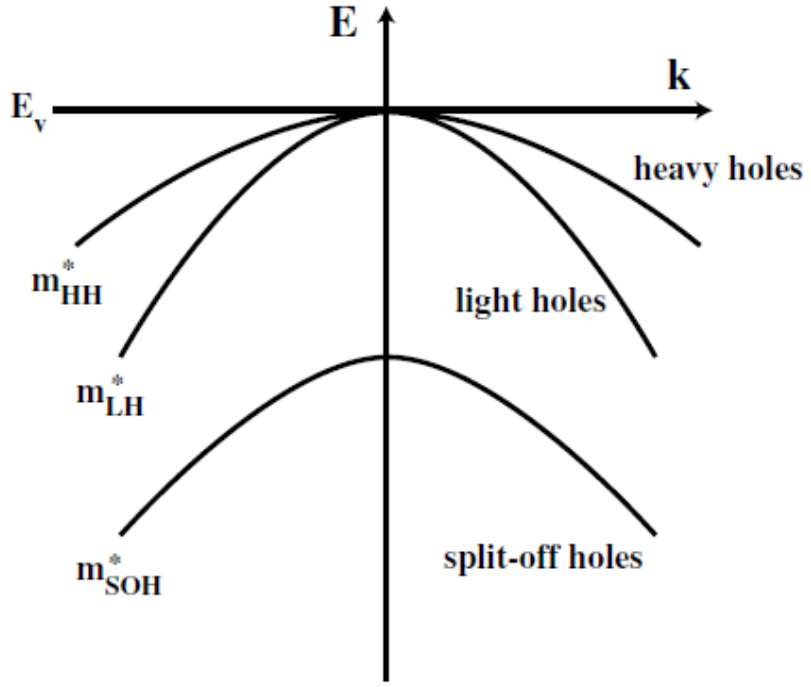
$$< \mathbf{L} \cdot \mathbf{S} > = \frac{1}{2} < \mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2 >$$

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

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

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

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

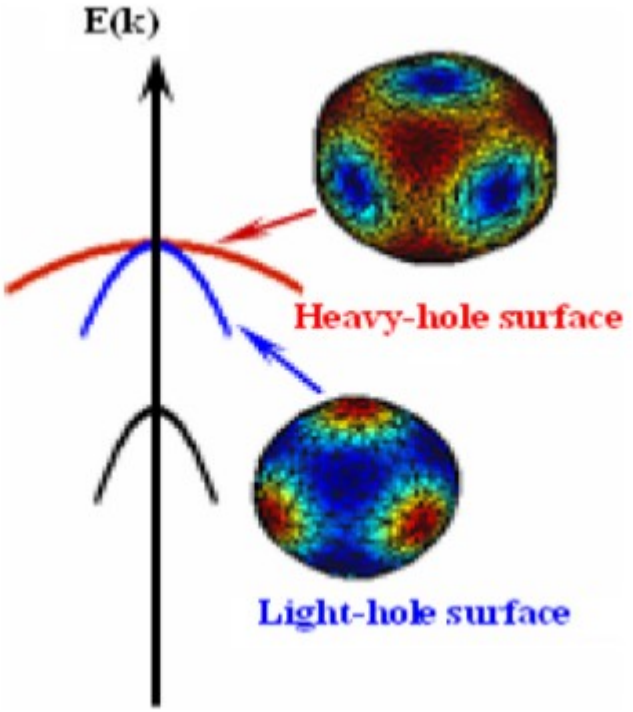
Split-off

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

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

Valence band structure

Isoenergy surfaces



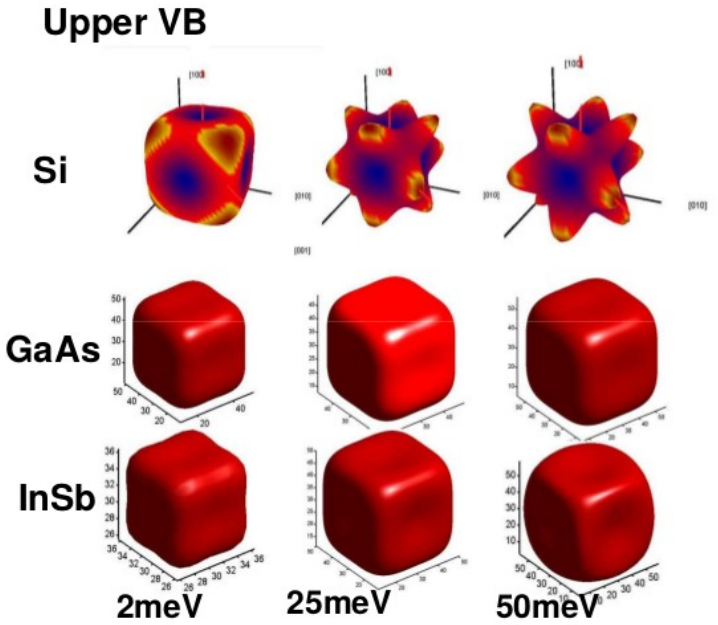


Figure 2 : Isoenergy surfaces for upper valence band in silicon, GaAs and InSb at 2meV / 25 meV / 50 meV.

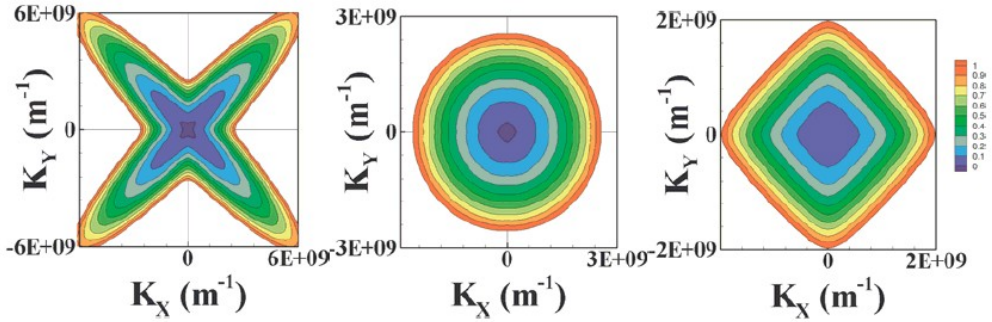
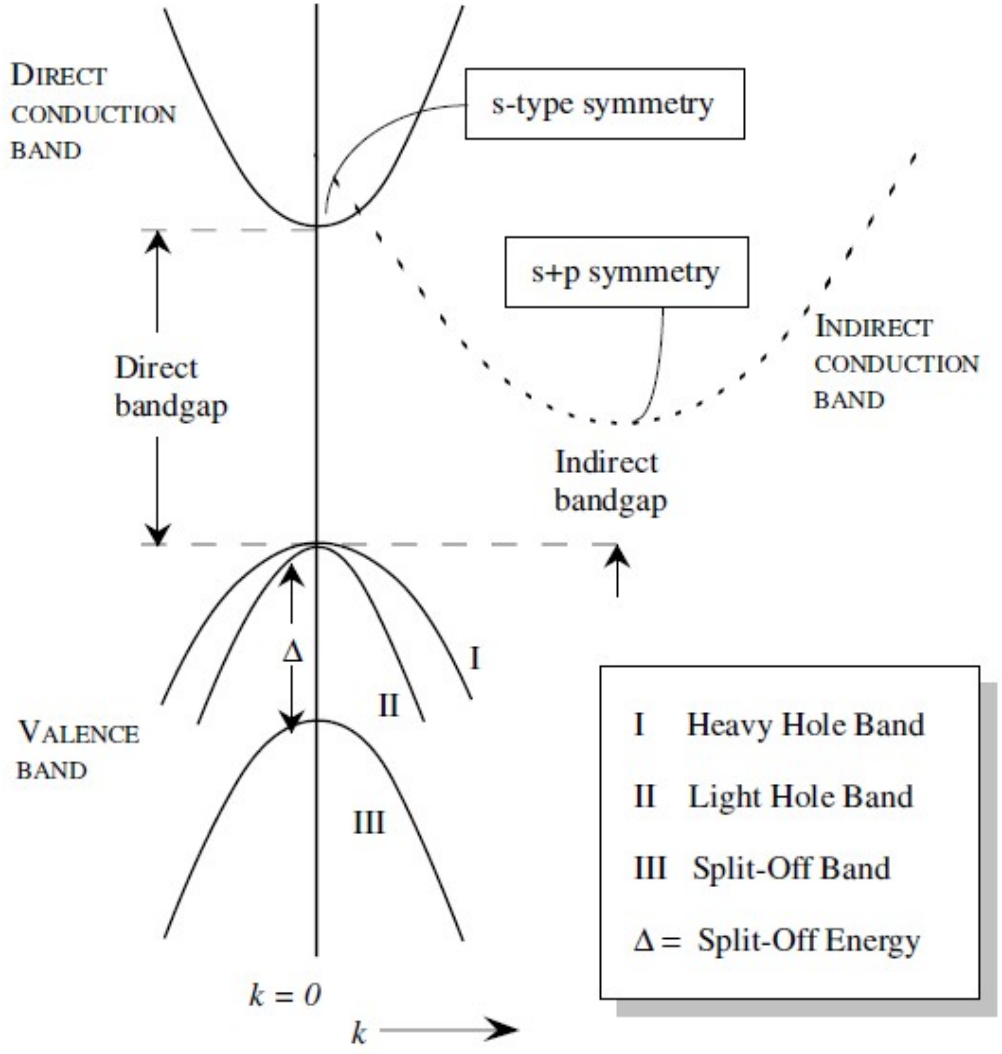


Figure 5. 3D equienergy surfaces of heavy hole, light hole and split off band in Si for $k_z = 0$.

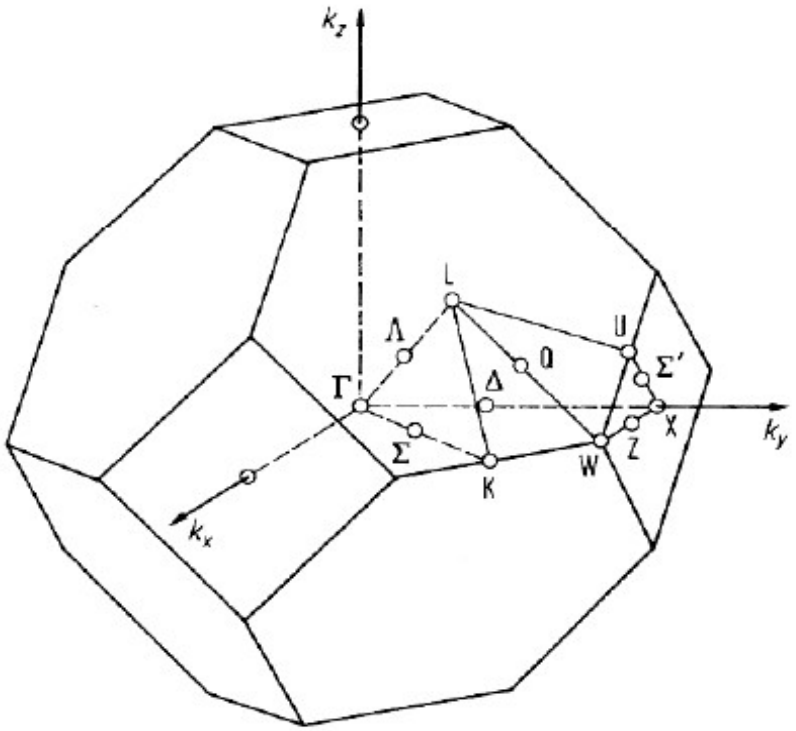
Valence band structure



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

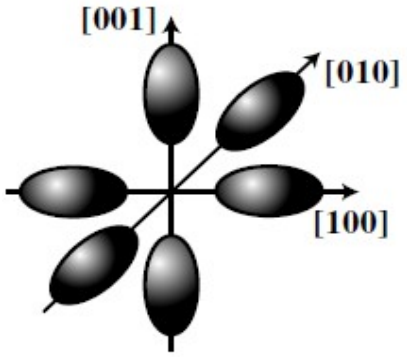
High symmetry points in semiconductors

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

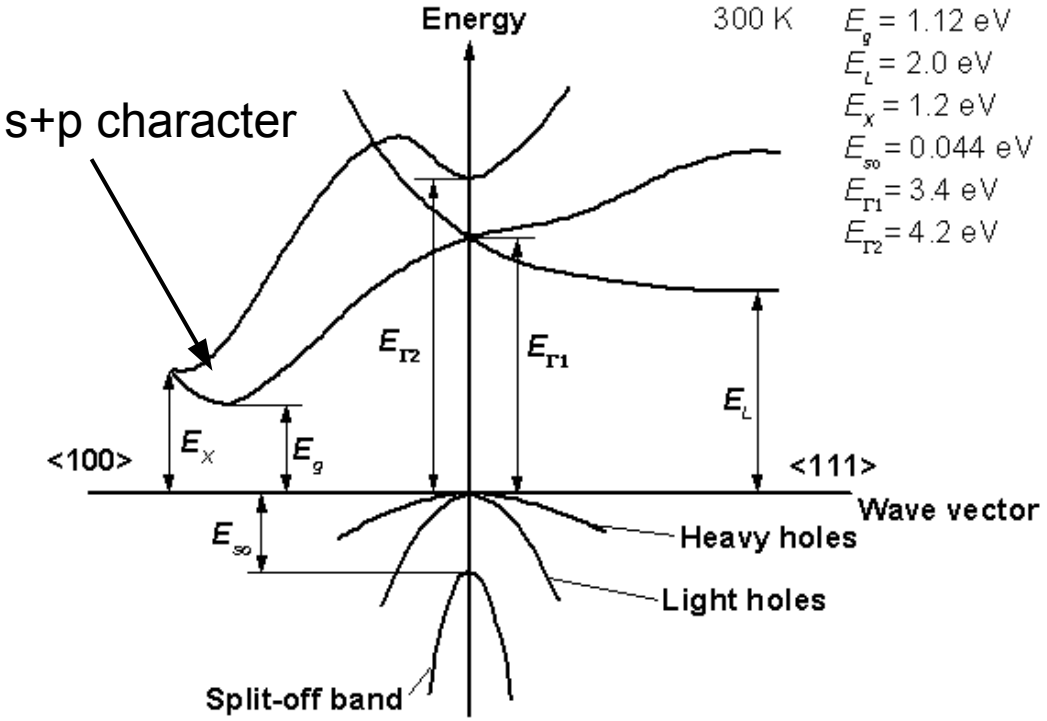


Silicon

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'.

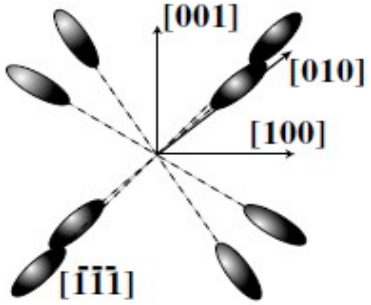


Position of the CB minima in reciprocal space

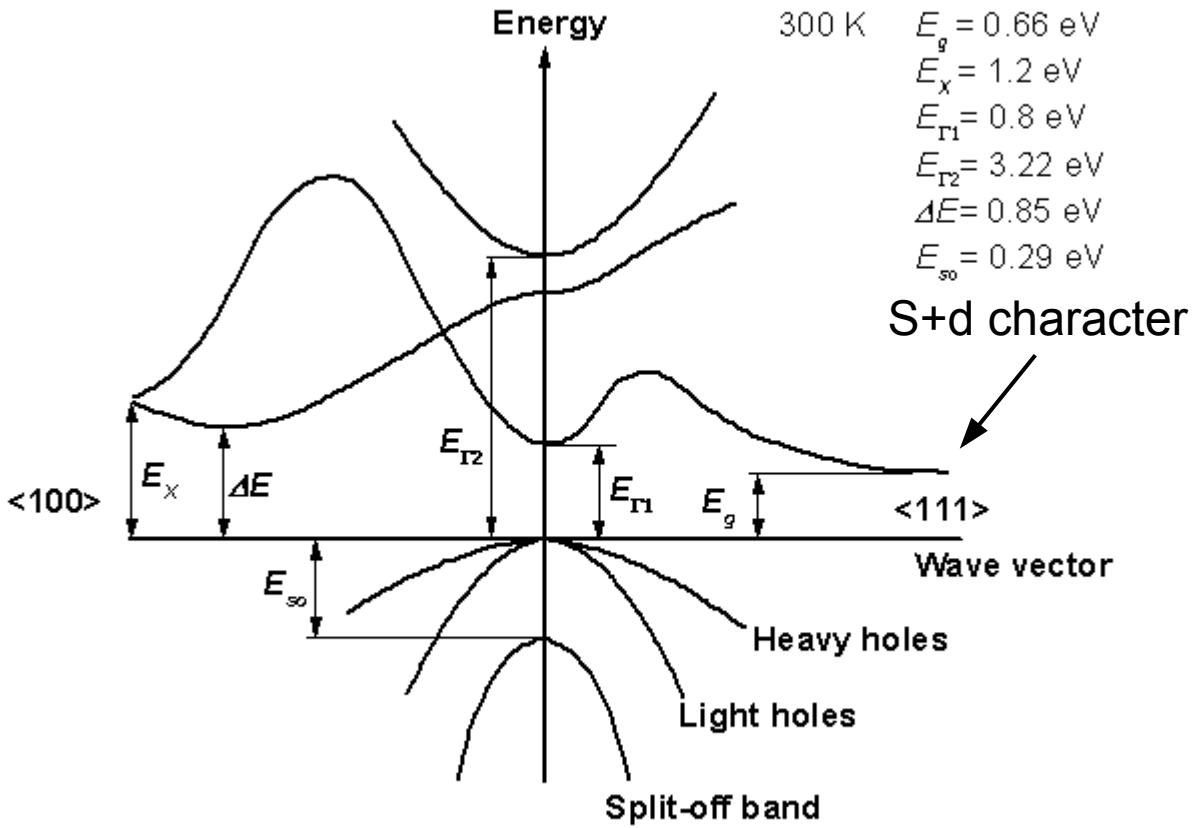


Germanium

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

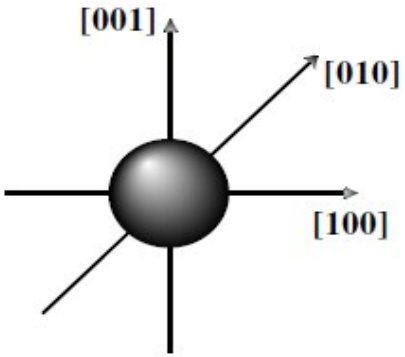


Position of the CB minima in reciprocal space

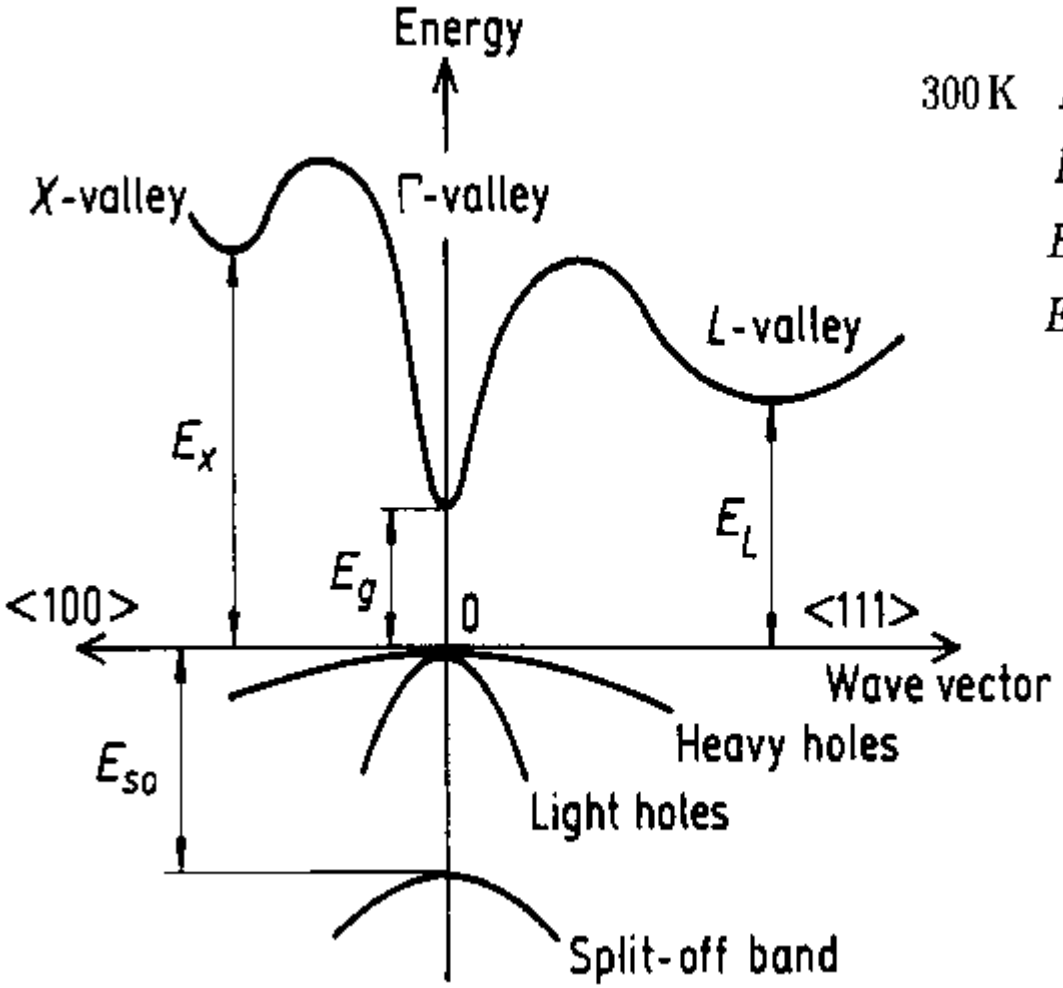


GaAs

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

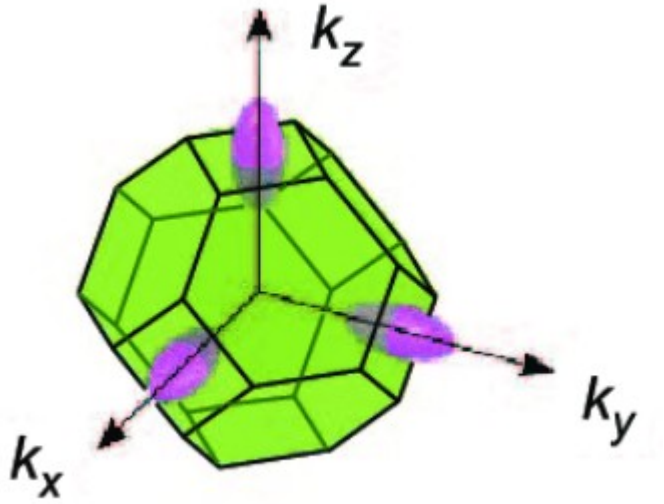


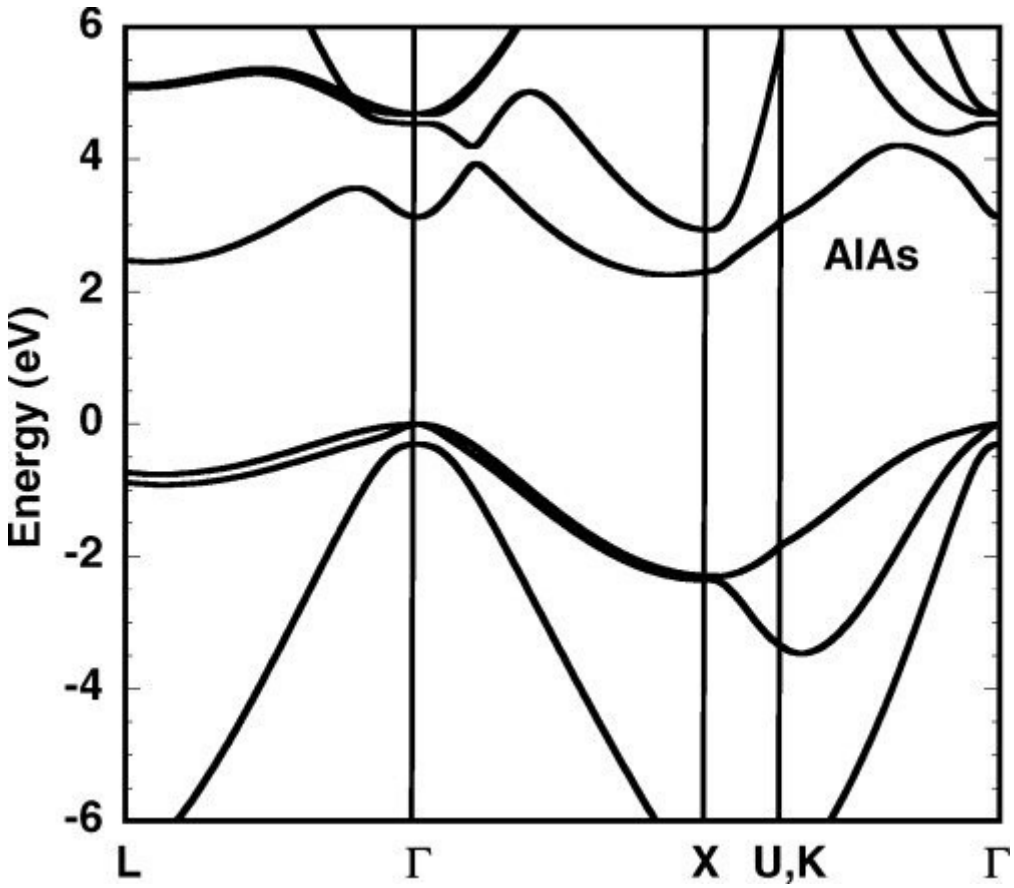
300 K $E_g = 1.42$ eV
$E_L = 1.71$ eV
$E_X = 1.90$ eV
$E_{so} = 0.34$ eV

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



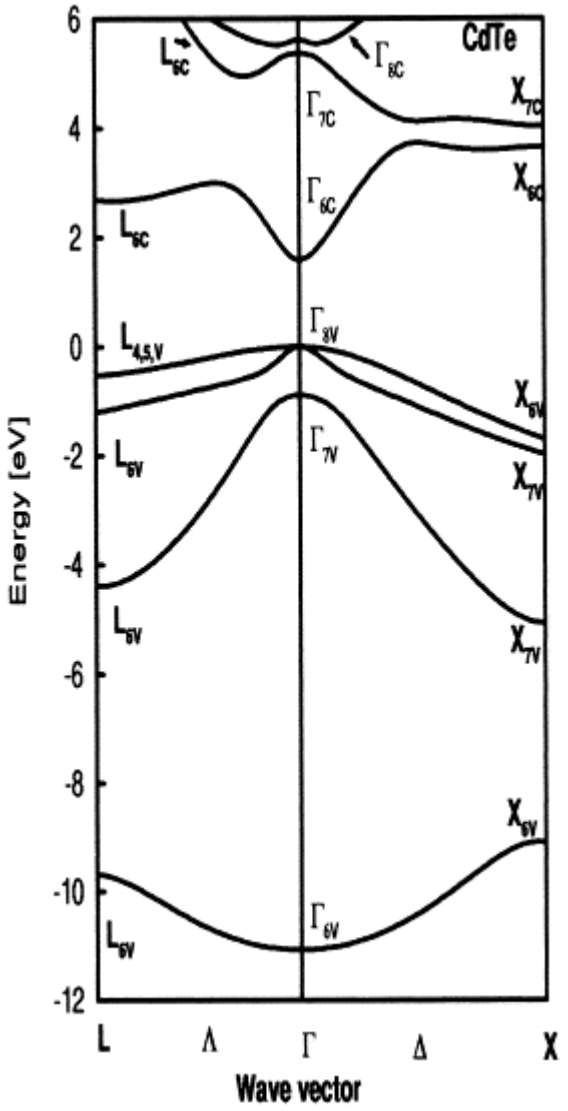


CdTe

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