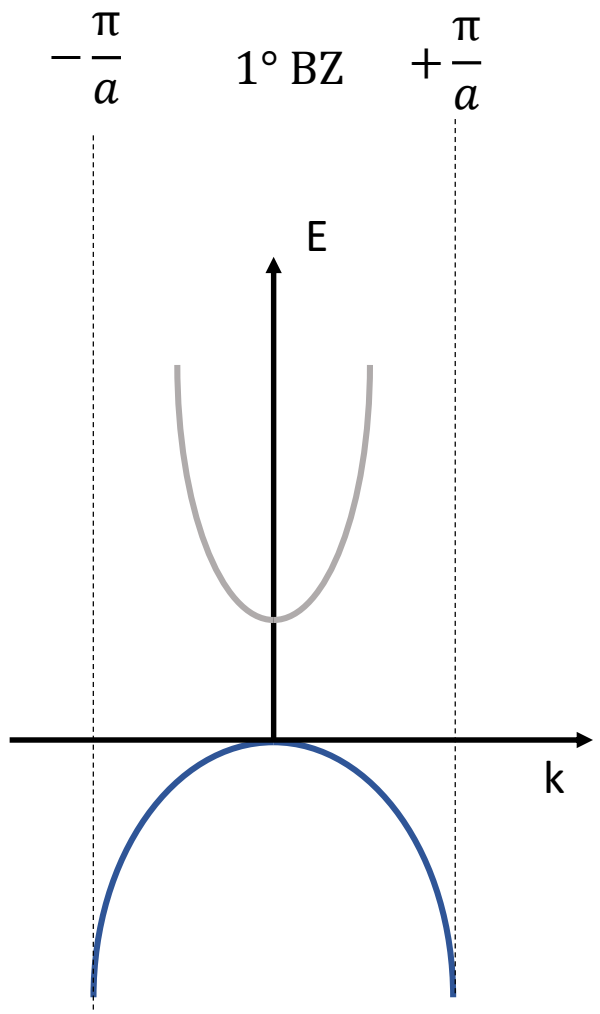
Class 03
Band Structures of real materials

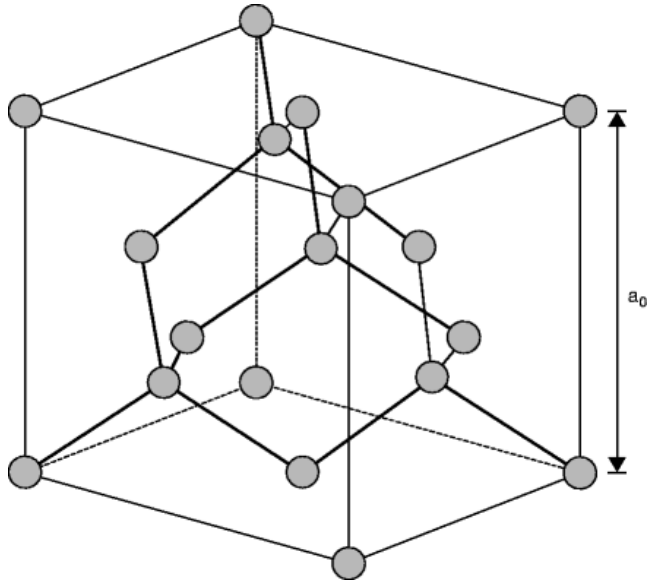
24.02.2025

- ❑ Crystal lattice and reciprocal space
  - Brillouin zone
  - Valence bands and split-off
- ❑ Exercise: Alloys
- ❑ Dispersion relationship in low-dimensional semiconductors
  - Particle in a box
  - Quantum well
- ❑ Band Structure and Density of States

Sketch vs real band structure

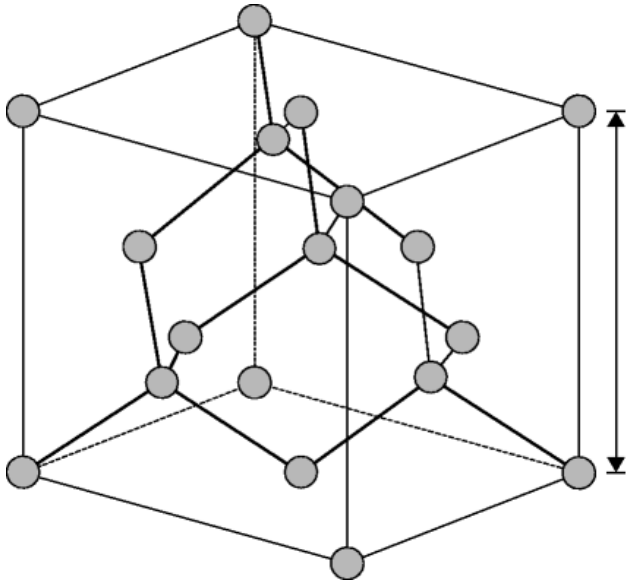


- Periodicity (unit cell)
- Reciprocal space (BZ)
- Atomic potential and energy gap
- Dispersion relationship
- Effective mass
- Electrons and holes



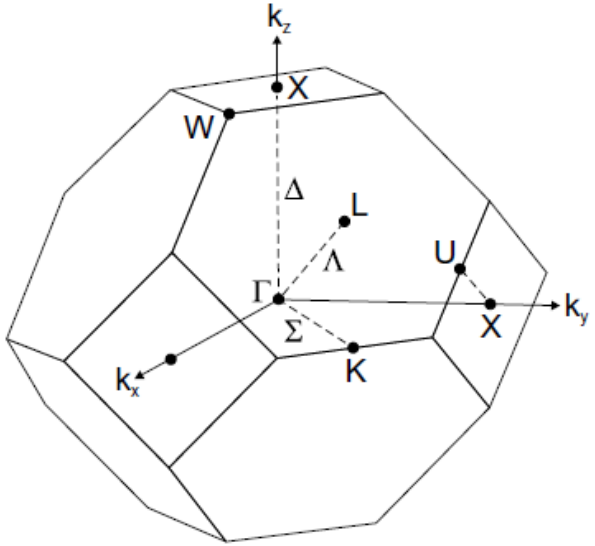
SILICON

Face Center Cubic (FCC)
Diamond Cubic



0.5431 nm

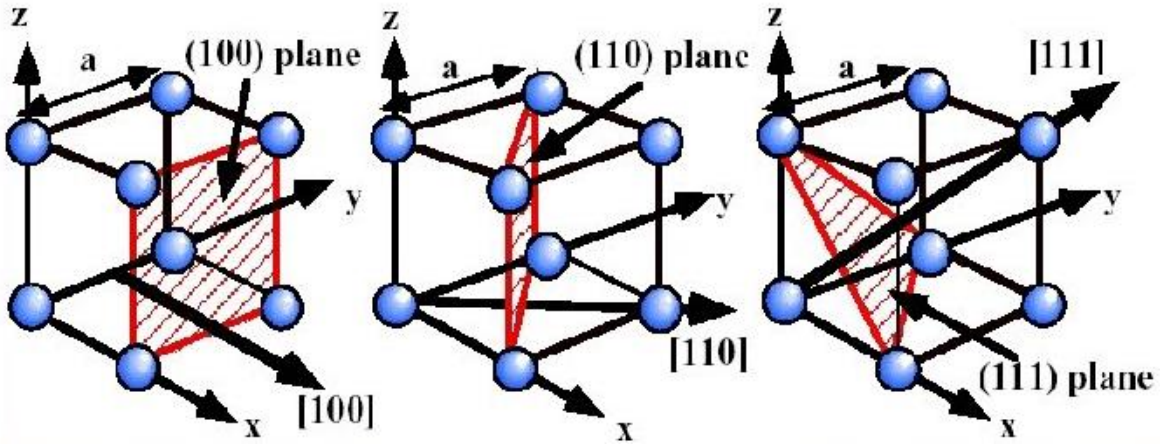
Brillouin Zone (Reciprocal Space)
Face Center Cubic (FCC)



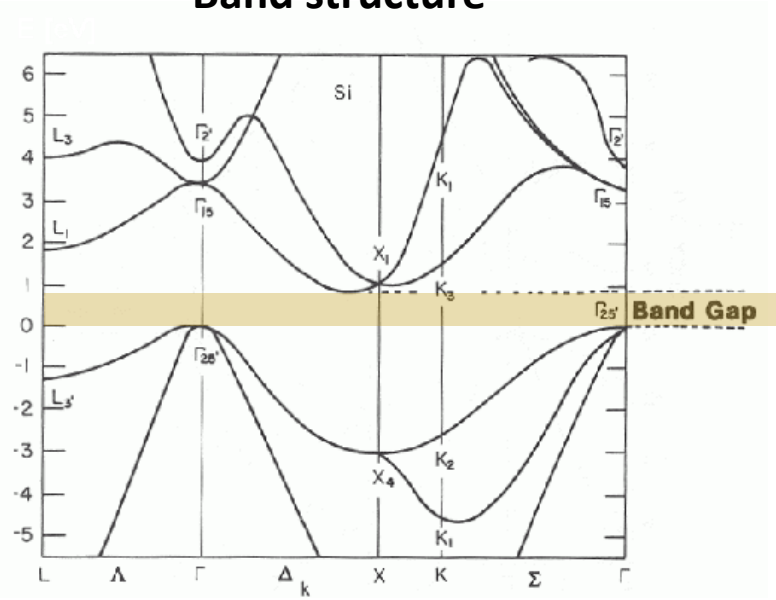
Γ = (000)
X = (001)
K = (110)
L = (111)

Grundmann 3.6

(100), (110), (111) crystal planes



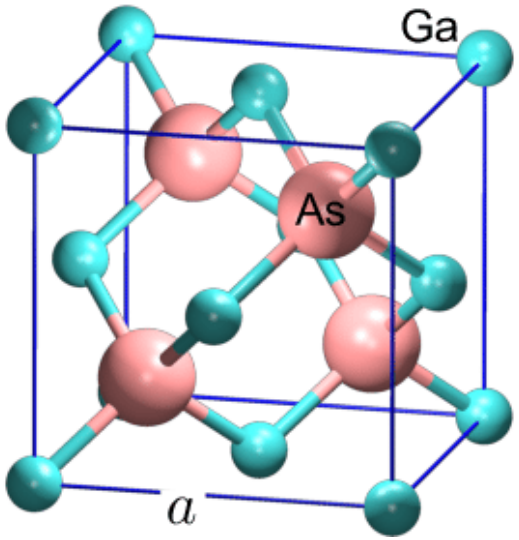
Band structure



1.12 eV

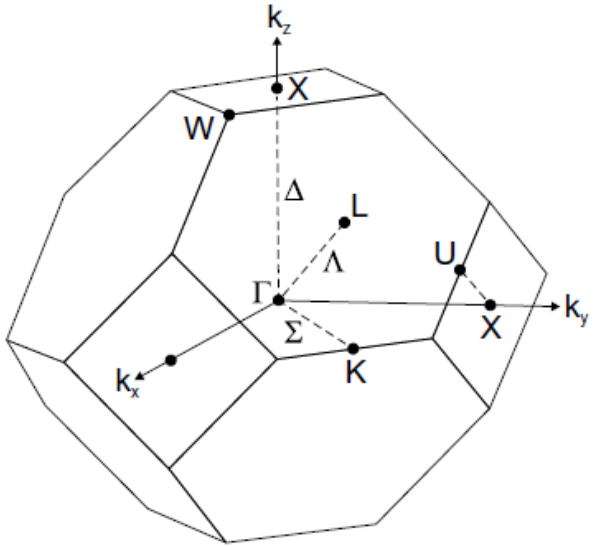
GaAs

Face Center Cubic (FCC)
Zinc blende



0.565nm

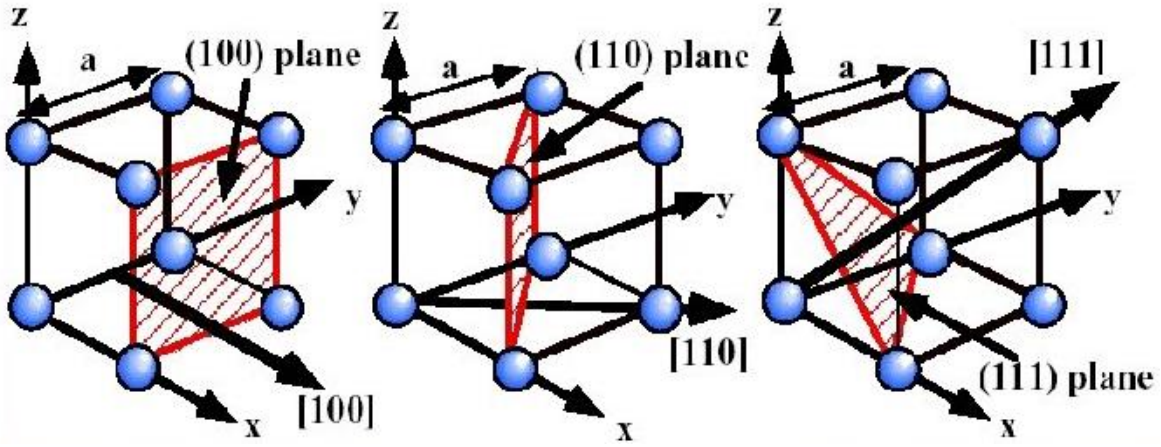
Brillouin Zone (Reciprocal Space)
Face Center Cubic (FCC)



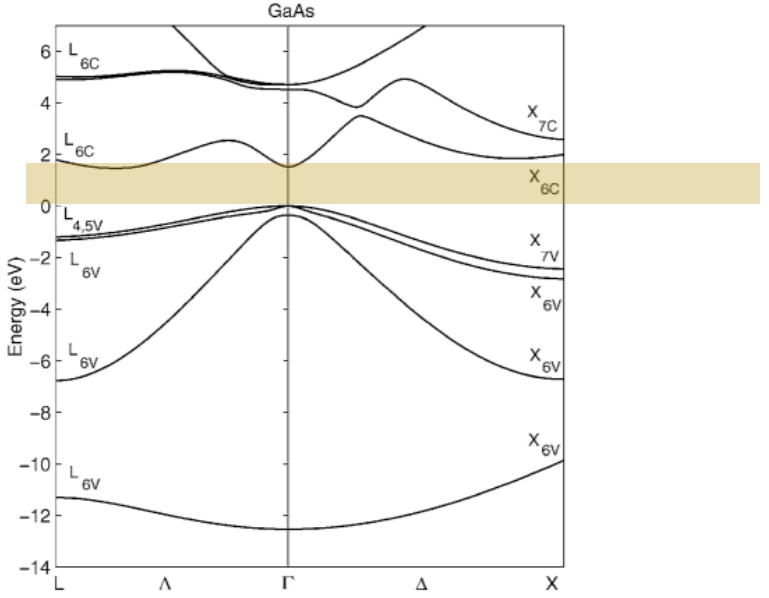
Γ = (000)
X = (001)
K = (110)
L = (111)

Grundmann 3.6

(100), (110), (111) crystal planes

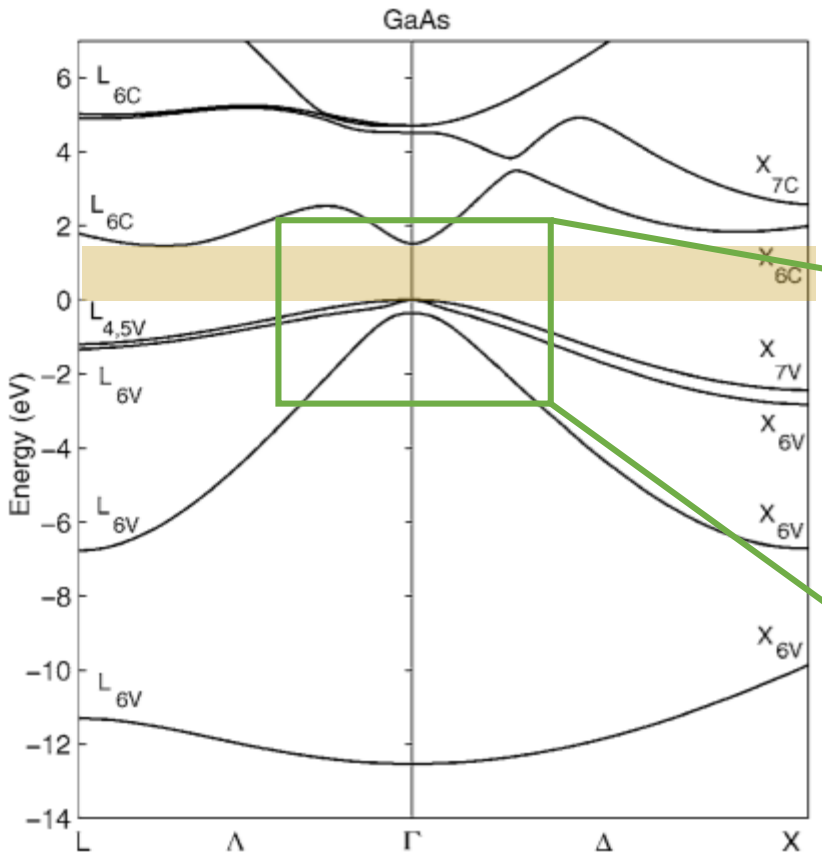


Band structure

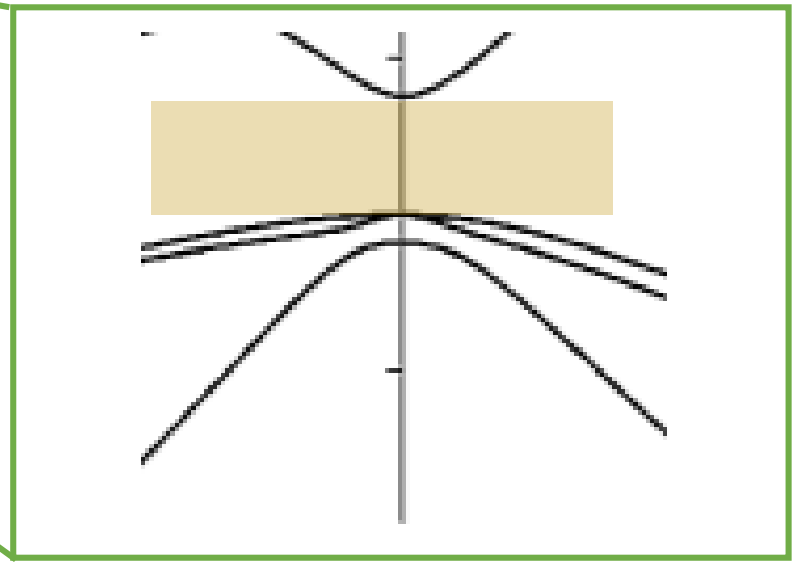


1.42 eV

Conduction and Valence bands in real materials



1.424 eV



1 Conduction band
3 Valence bands

Valence bands in zinc-blende lattices

l = 1
s = ±1/2
j = 3/2 or 1/2 (2-degenerate)

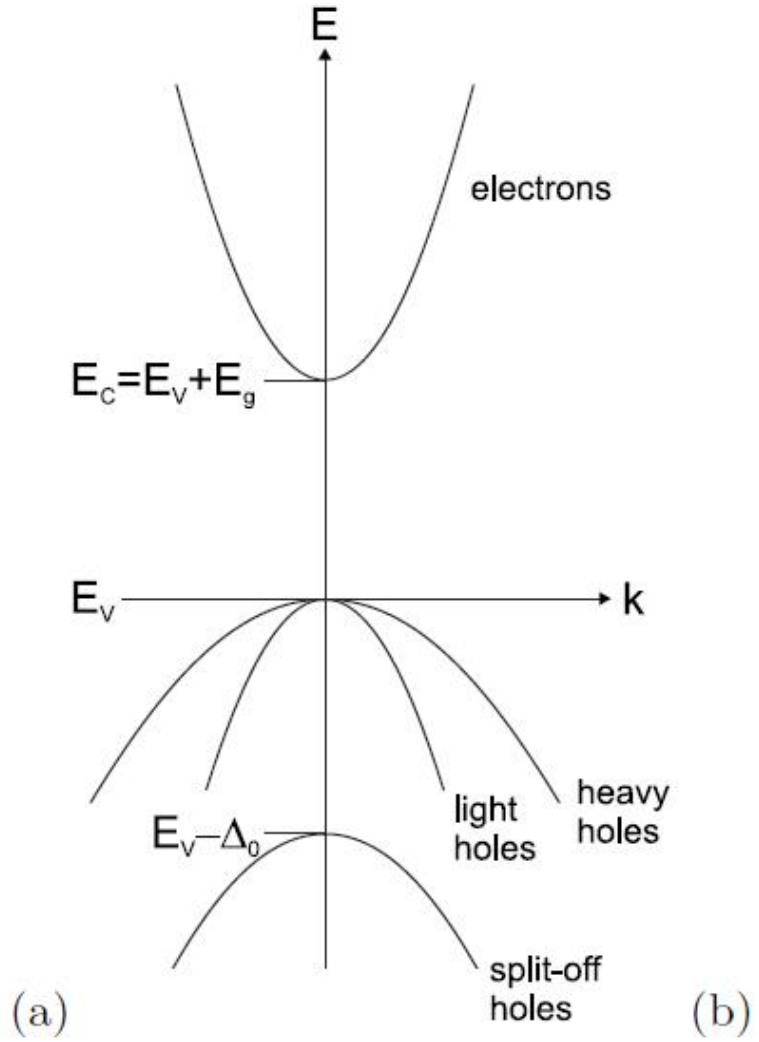
Heavy holes

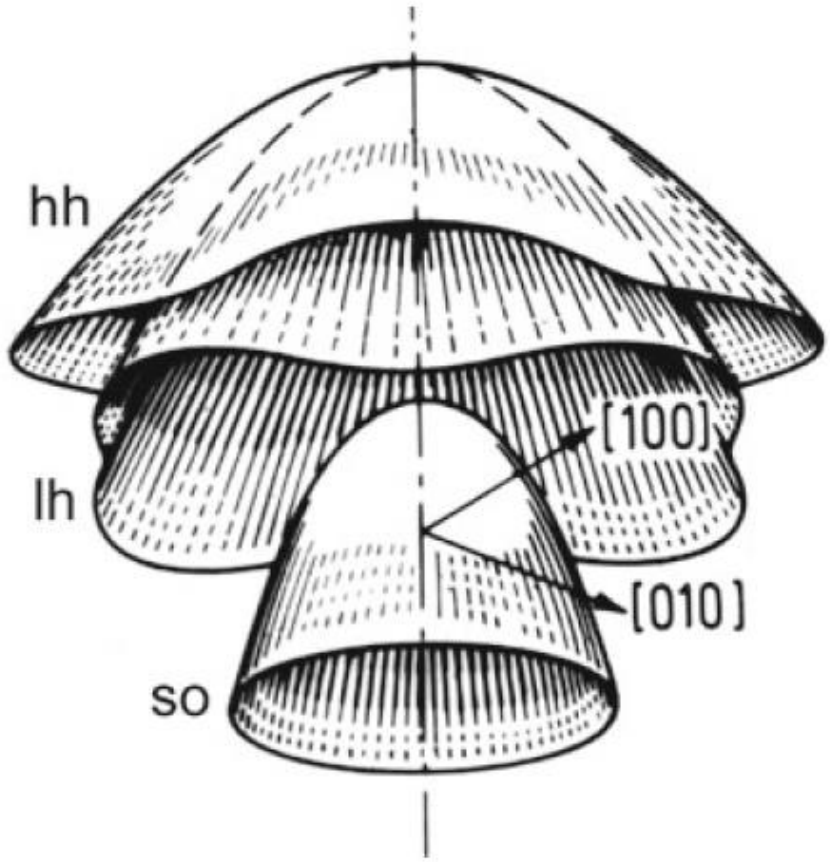
Light holes

Split-off holes

The split-off energy Δ_0 arises from the interaction of the atomic angular momentum and the electron spin.

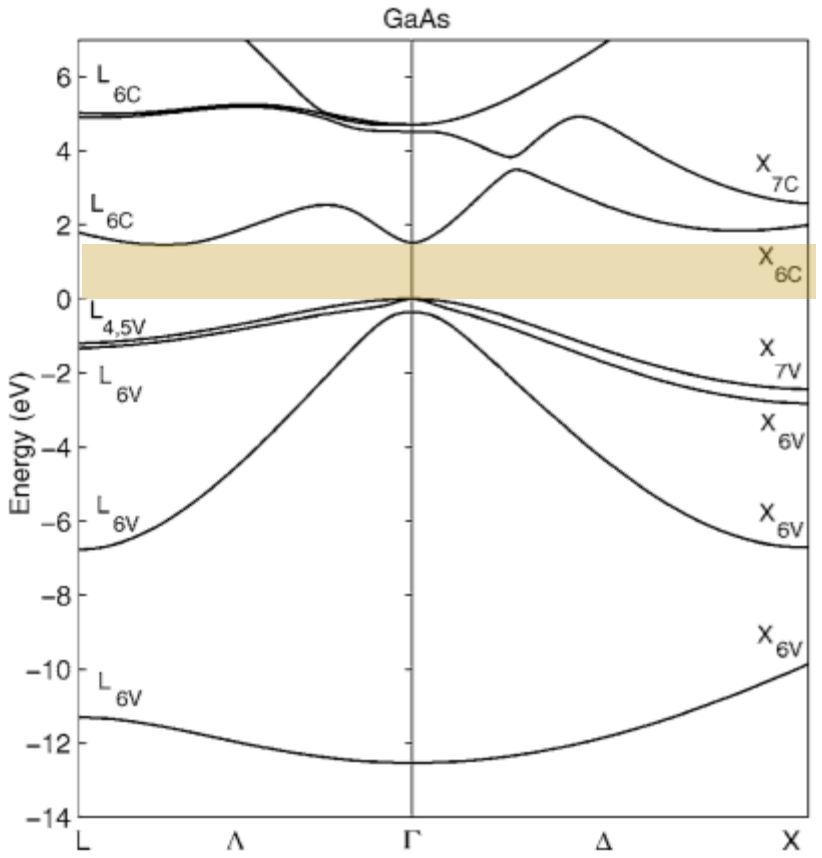
Materials with high spin-orbit interaction have high Δ_0 values.



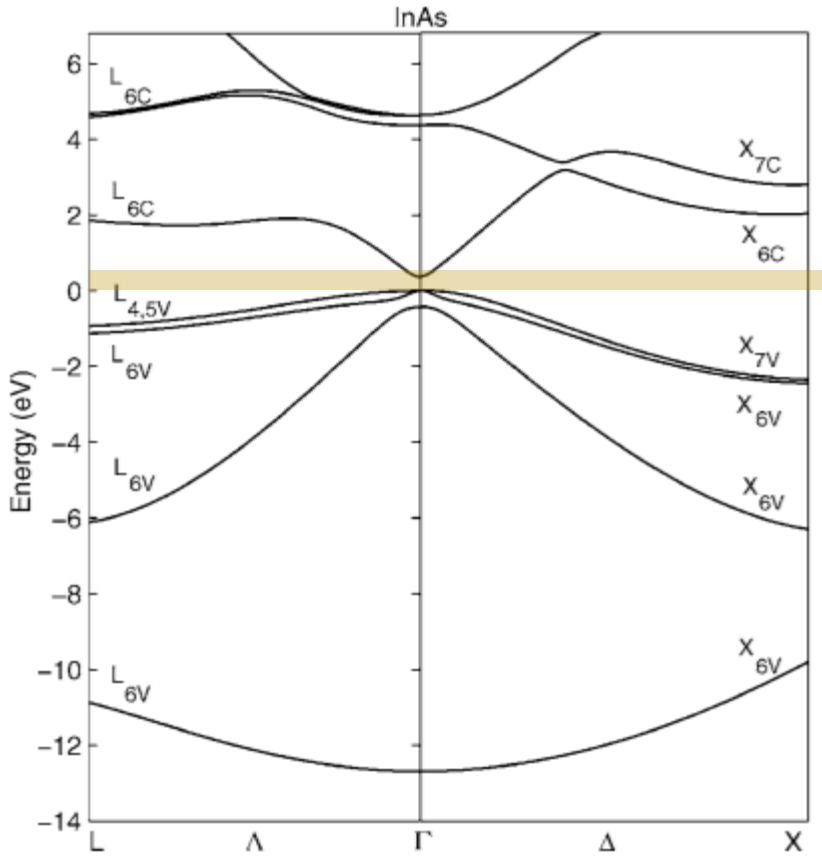


Valence bands in Ge

In-Class Exercise



1.424 eV



0.354 eV

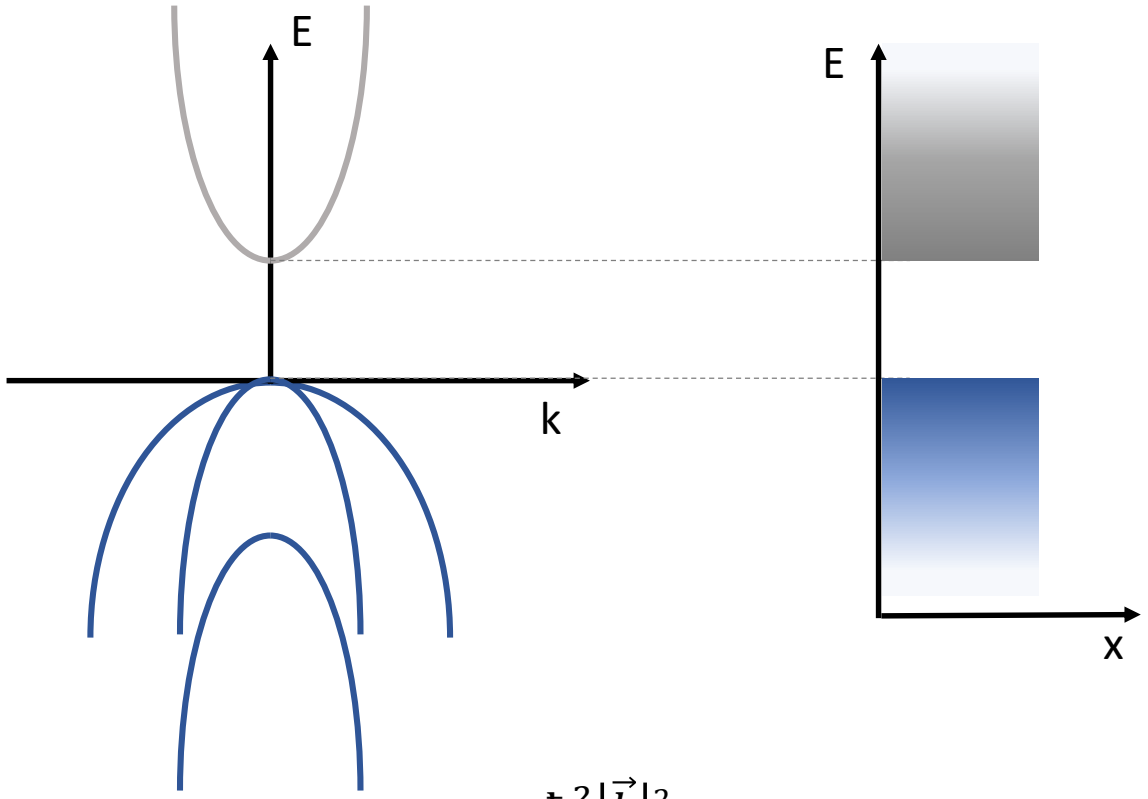
Could you write the function to calculate the band gap of the ternary alloy $In_{(1-x)}Ga_{(x)}As$?

10 minutes

To be discussed in Class

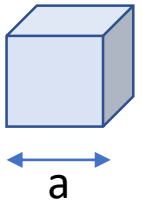
Band structure in quantum dots

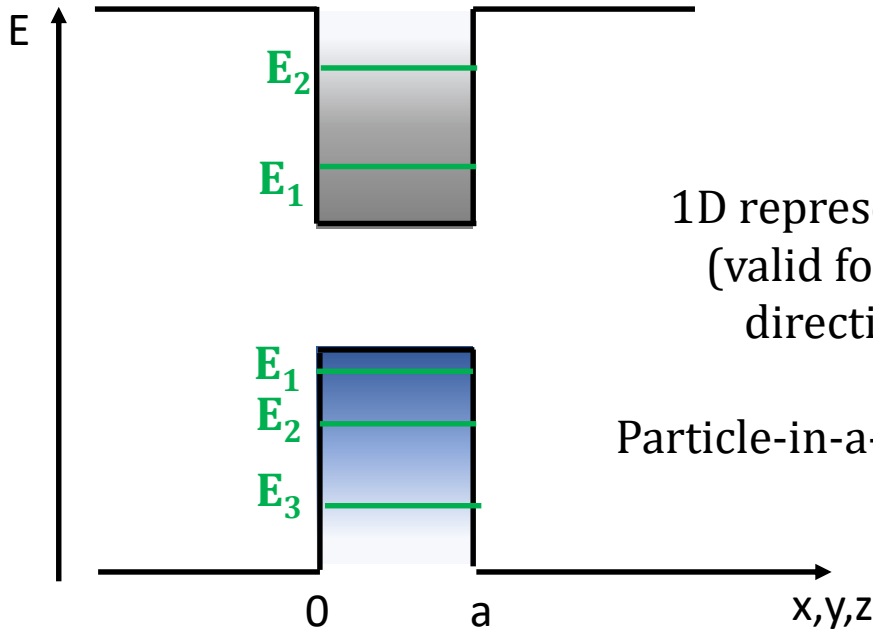
E(k) relation in bulk



$$E = \frac{\hbar^2 |\vec{k}|^2}{2m^*}$$

Energy levels in 0D





1D representation (valid for the 3 directions)

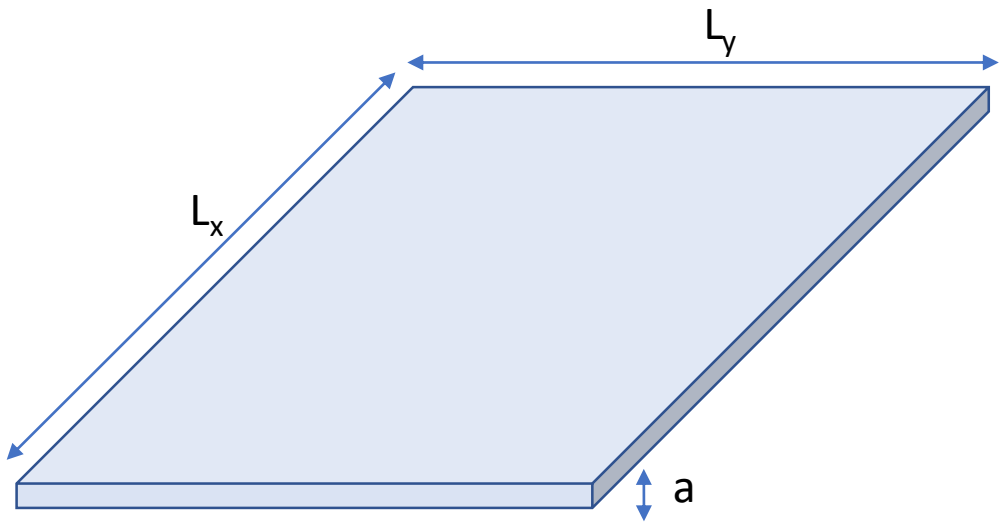
Particle-in-a-box model

$$E_n = \frac{\hbar^2 |k_n|^2}{2m^*} \qquad where\ k_n = \frac{n * \pi}{a}$$

Homework:

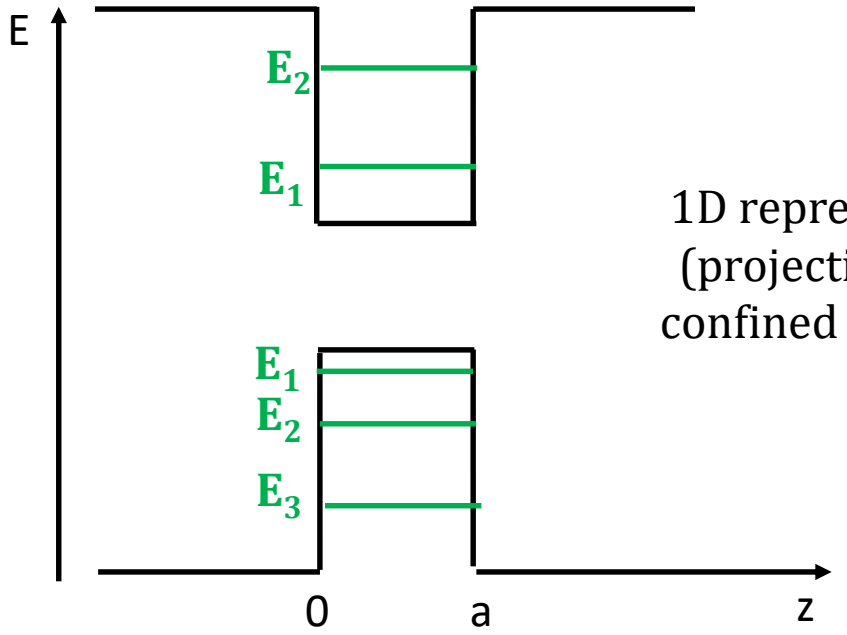
The sketch contains 3 discrete levels in the valence band and only 2 in the conduction band: why?

Band structure in quantum wells



$Lx, Ly \gg a$

Energy levels in 2D

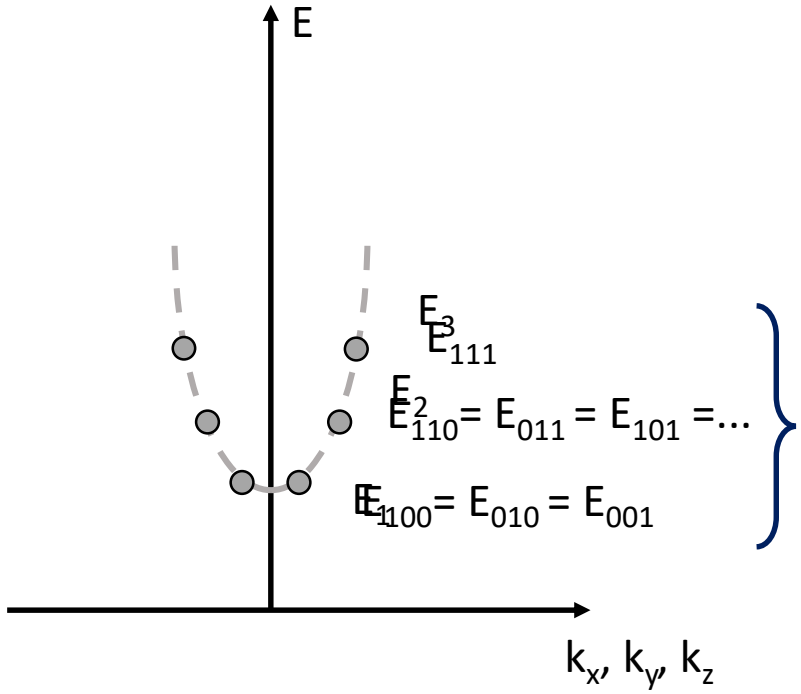


1D representation (projection in the confined direction)

$$E_n = \frac{\hbar^2 |k_n|^2}{2m^*} \quad where\ k_n = \frac{n * \pi}{a}$$

E(k) in quantum dots and wells

0D

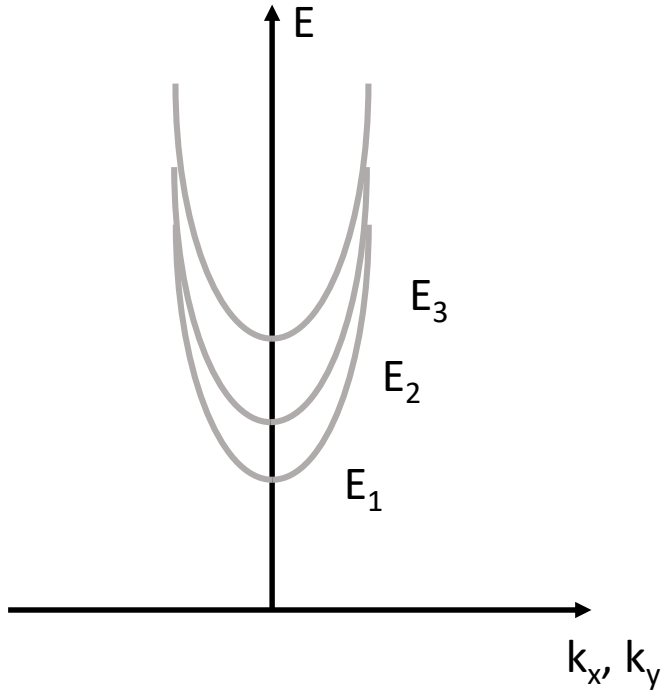


Equivalence are correct if:
$a_x = a_y = a_z$

$$E_{n,m,l} = \frac{\hbar^2 |k_{n,m,l}|^2}{2m^*}$$

$$|k_{n,m,l}|^2 = \left(\frac{n * \pi}{a_x}\right)^2 + \left(\frac{m * \pi}{a_y}\right)^2 + \left(\frac{l * \pi}{a_z}\right)^2$$

2D



$$E_{n,x,y} = \frac{\hbar^2 |k_{n,x,y}|^2}{2m^*}$$

$$|k|^2 = k_x^2 + k_y^2 + k_n^2$$

$$k_n^2 = \left(\frac{n * \pi}{a_z}\right)^2$$

Homework:

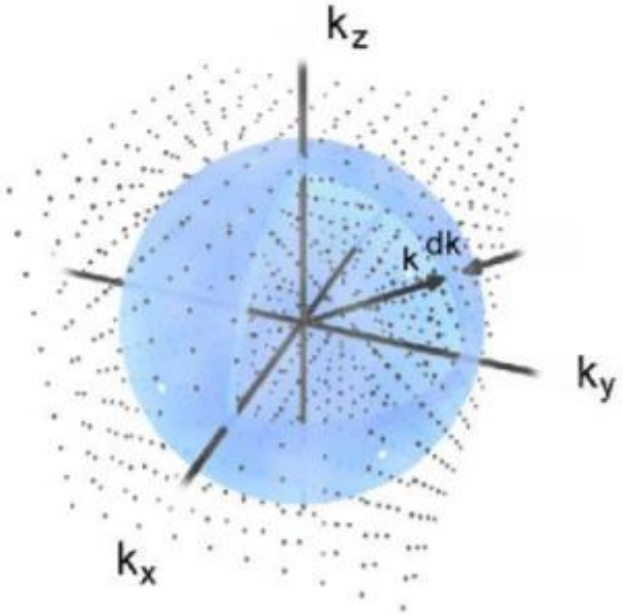
Sketch the E(k) relation in the case of a quantum wire (1D)

Density of states in 3D

The density of space g(E) is the number of states available in the material with energy between E and E+ΔE

To compute it, it is necessary to understand how many k states are present in the reciprocal states. In 3D, the k states in the reciprocal space can be expressed as:

$$k = \frac{\pi^3}{L_x L_y L_z}$$



More details in Grundmann, 6.13.3

The density of k states can be expressed as a quarter-spherical relation, including the spin-degeneracy:

$$g(k)dk = \underbrace{2}_{\text{Spin-degeneracy}} * \underbrace{\frac{1}{8} * \frac{V}{\pi^3}}_{\text{Volume of a single state}} * \underbrace{4 * \pi k^2\, dk}_{\text{Volume of a slice of sphere in k-space}}$$

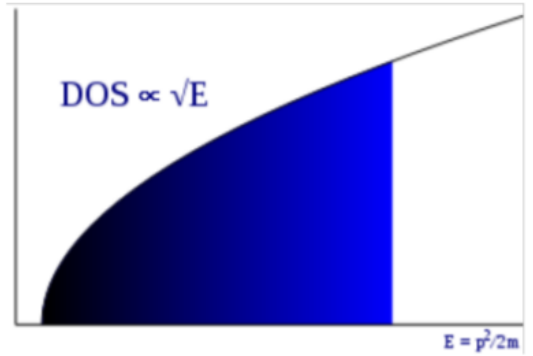
The density of k states can therefore be expressed as:

$$g(k)dk = \pi k^2 \left[\frac{V}{\pi^3}\right] dk = \left[\frac{V k^2}{\pi^2}\right] dk$$

Using the quantum-mechanical and the dispersion relationships:

$$p = \hbar k\,,\; E = p^2/2m^* \quad E = \frac{\hbar^2 k^2}{2m^*}$$

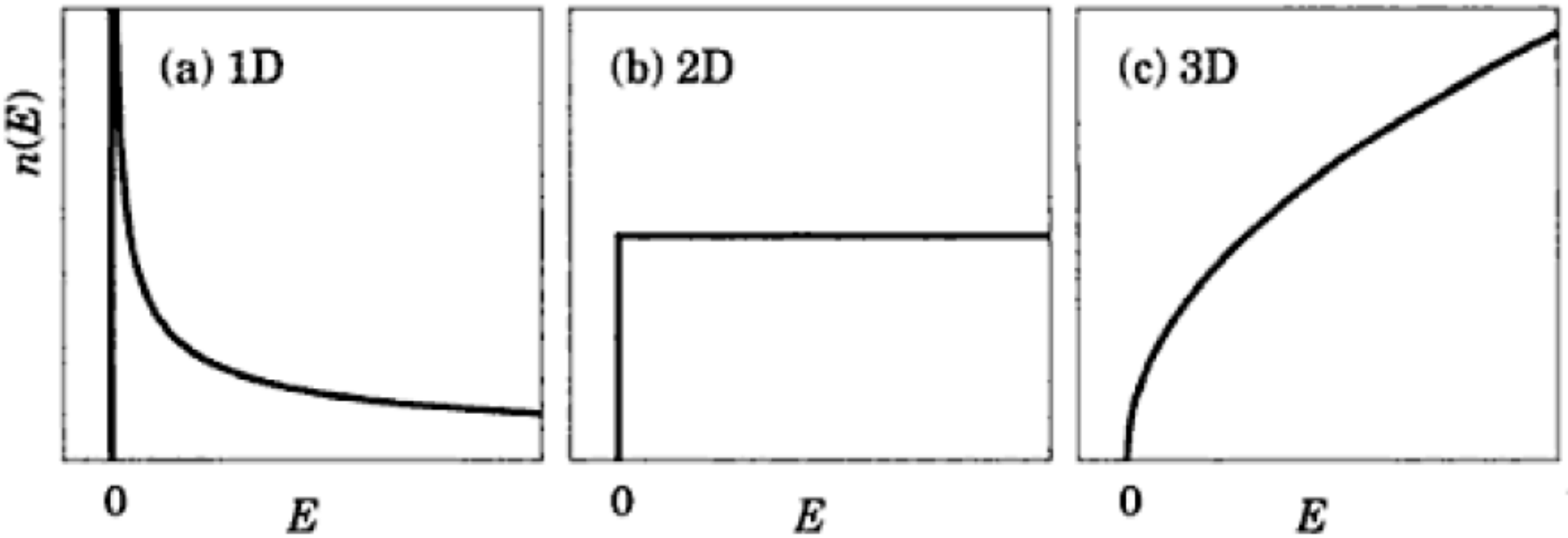
$$g(E)dE = \frac{m^*\left[2m^*(E-E_c)\right]^{1/2}}{\pi^2\hbar^3} dE$$



3-D density of states, which are filled in order of increasing energy.

g(E) α $\sqrt{E}$

Density of states in low D



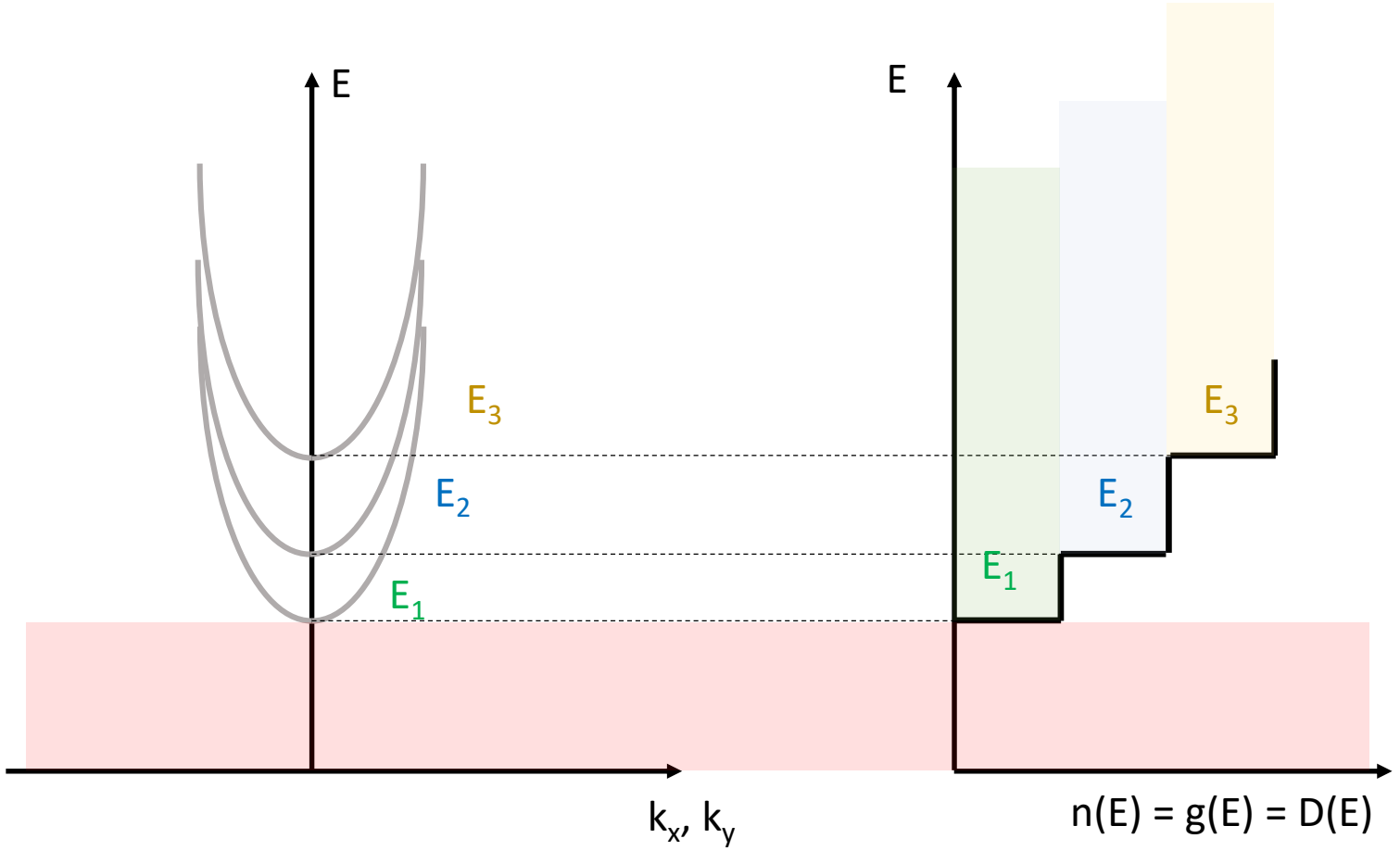
The density of states in nanostructures varies with the dimensionality.

In 3D: g(E) α $\sqrt{E}$
In 2D: g(E) = const
In 1D: g(E) α $1/\sqrt{E}$

Homework:
Try to compute the DOS in 2D and 1D. How does the DOS look like in the case of a quantum dot (0D)?

Dispersion relationship vs DOS

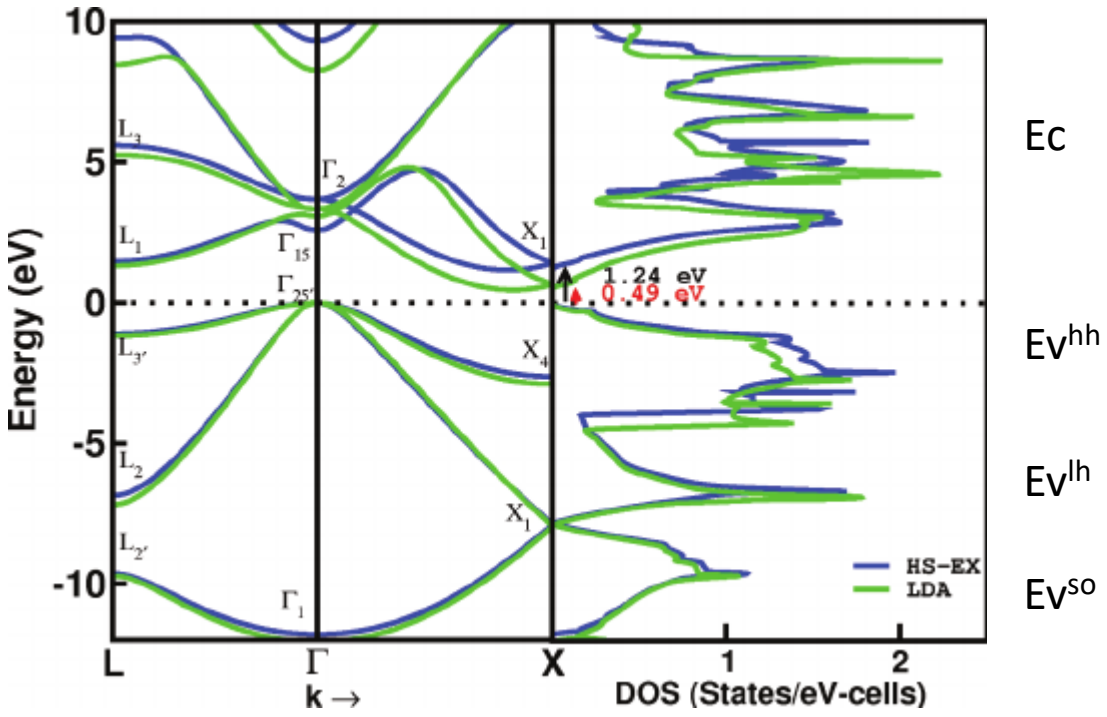
Example: 2D



Question:

In light of the DOS, explain why some devices (photodetectors, LEDs) are expected to work more efficiently in 1D form.

SILICON



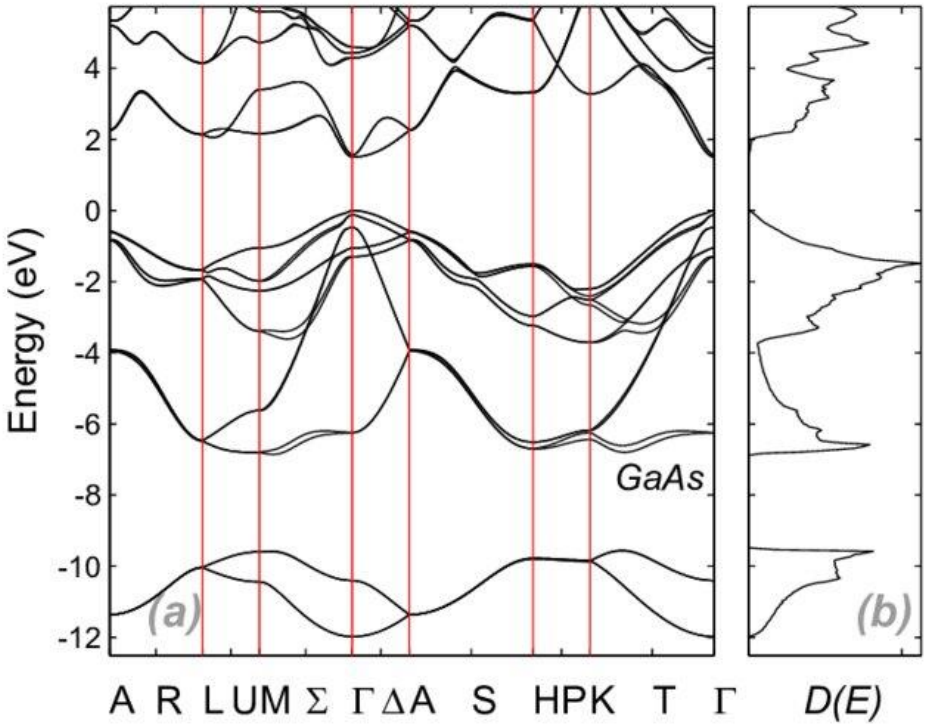
Ec

Ev^{hh}

Ev^{lh}

Ev^{so}

GaAs



Ec

Ev^{hh}

Ev^{lh}

Ev^{so}