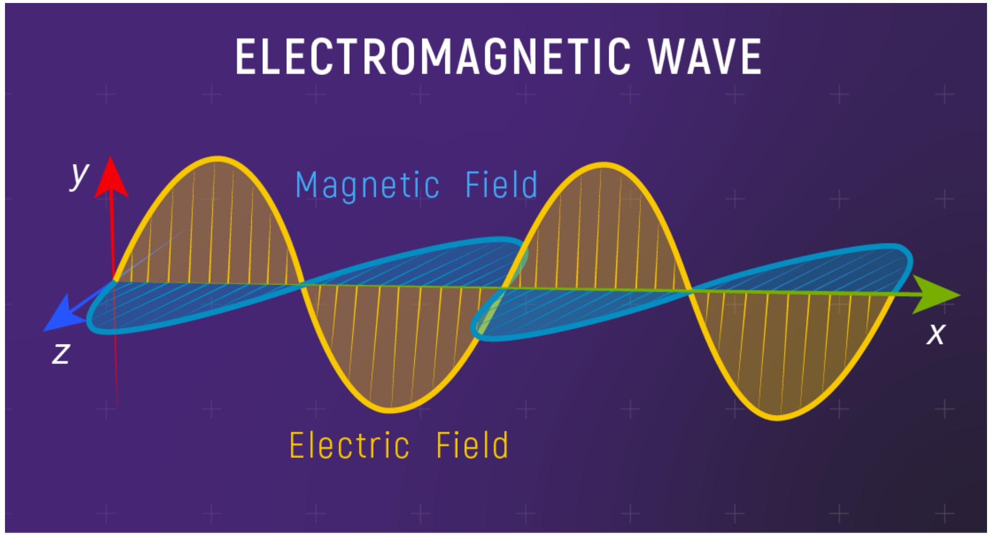
Class 06
Optical properties of semiconductors

11.03.2025

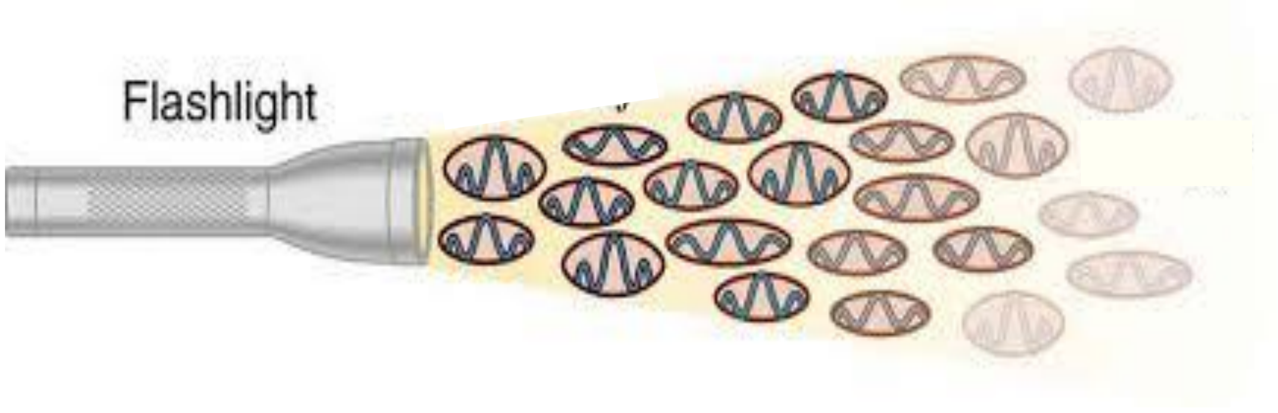
- Absorption coefficient
  - Direct semiconductors
  - Indirect semiconductors
  - Tauc plot

- Optical phenomena in real crystals
  - Urbach tail
  - Amorphous vs crystalline
  - Excitons

Wave-particle dual nature



$wavelength\ (\lambda)$



$$E = \frac{hc}{\lambda} = h\nu = \hbar\omega$$

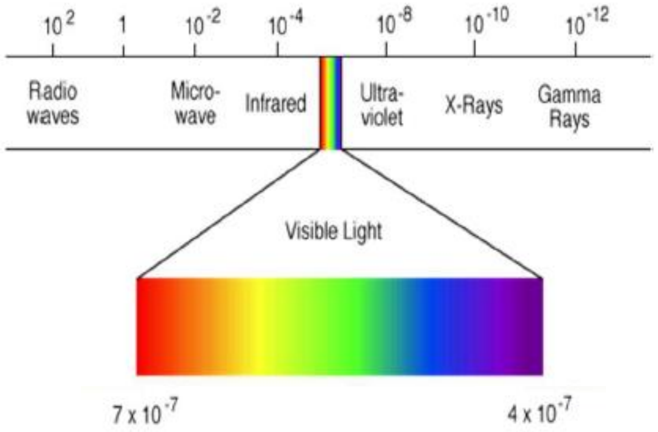


Table 9.1 Spectral ranges with relevance to semiconductor optical properties

Range		Wavelengths	Energies
Deep ultraviolet	DUV	<250 nm	>5 eV
Ultraviolet	UV	250–400 nm	3–5 eV
Visible	VIS	400–800 nm	1.6–3 eV
Near infrared	NIR	800 nm–2 µm	0.6–1.6 eV
Mid-infrared	MIR	2–20 µm	60 meV–0.6 eV
Far infrared	FIR	20–80 µm	1.6–60 meV
THz region	THz	>80 µm	<1.6 meV

Light absorption

Light propagation in vacuum

$$E(z,t) = E_0 * \exp[i(kz - \omega t)] \qquad where\ k = \frac{\omega}{c}$$

Propagation velocity in an absorbing medium

$$v_p = \frac{c}{\check{n}} \qquad k = \frac{\check{n}\omega}{c} \qquad where\ \check{n} = n + i\kappa$$

Complex refractive index

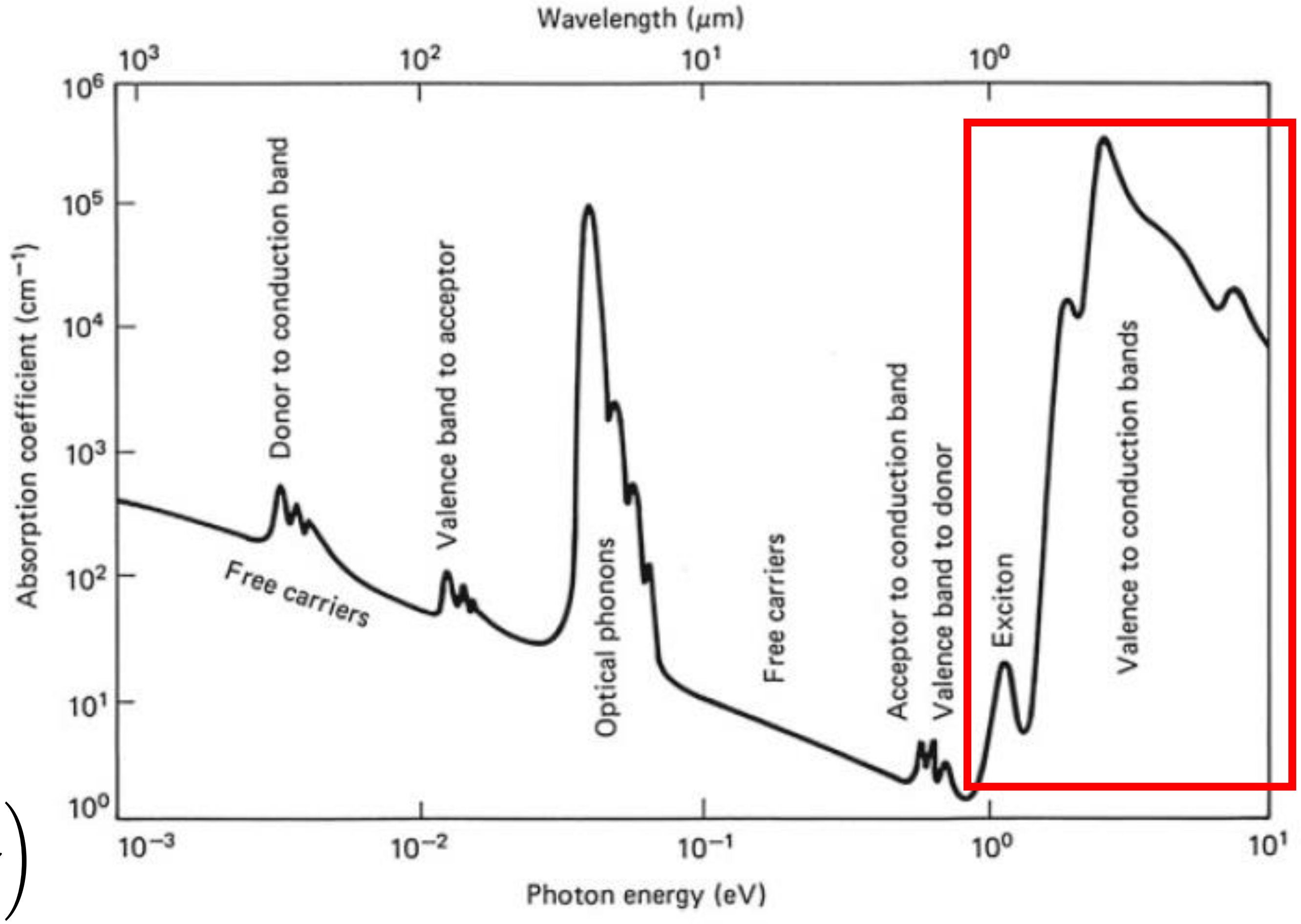
Light propagation in an absorbing medium

$$E(z,t) = E_0 * \exp\left(-\frac{\kappa\omega}{c}z\right) * \exp\left[i\left(\frac{n\omega}{c}z - \omega t\right)\right]$$

$$I(z) = |E|^2 = |E_0|^2 * \exp\left(-\frac{2\kappa\omega}{c}z\right) = I_0 * exp\left(-\frac{2\kappa\omega}{c}z\right)$$

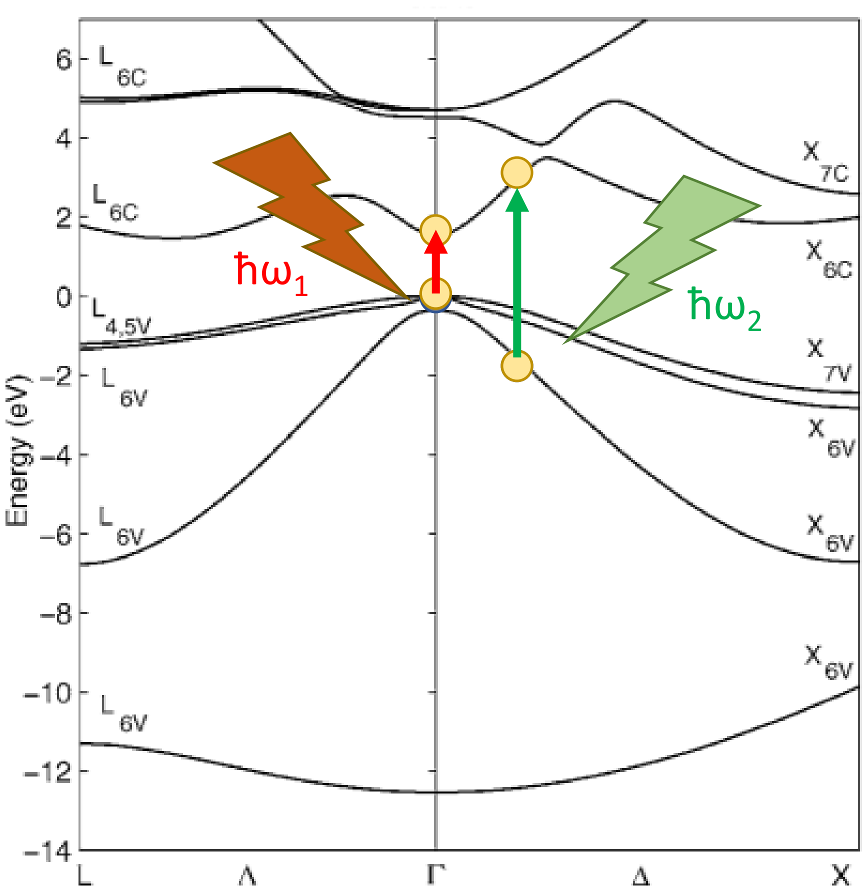
$$\boldsymbol{I(z) = I_0 * exp(-\alpha z)}$$

Lambert-Beer's law



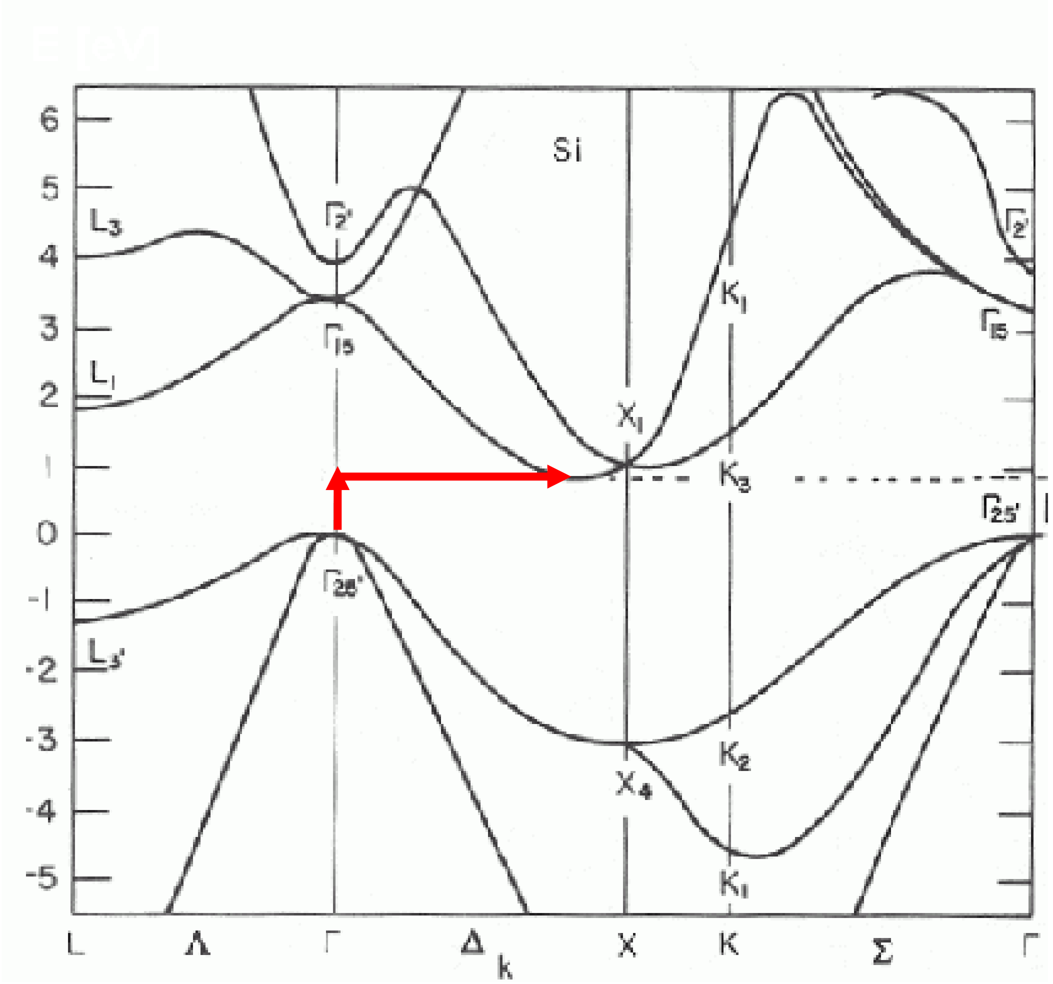
Band to band absorption

GaAs



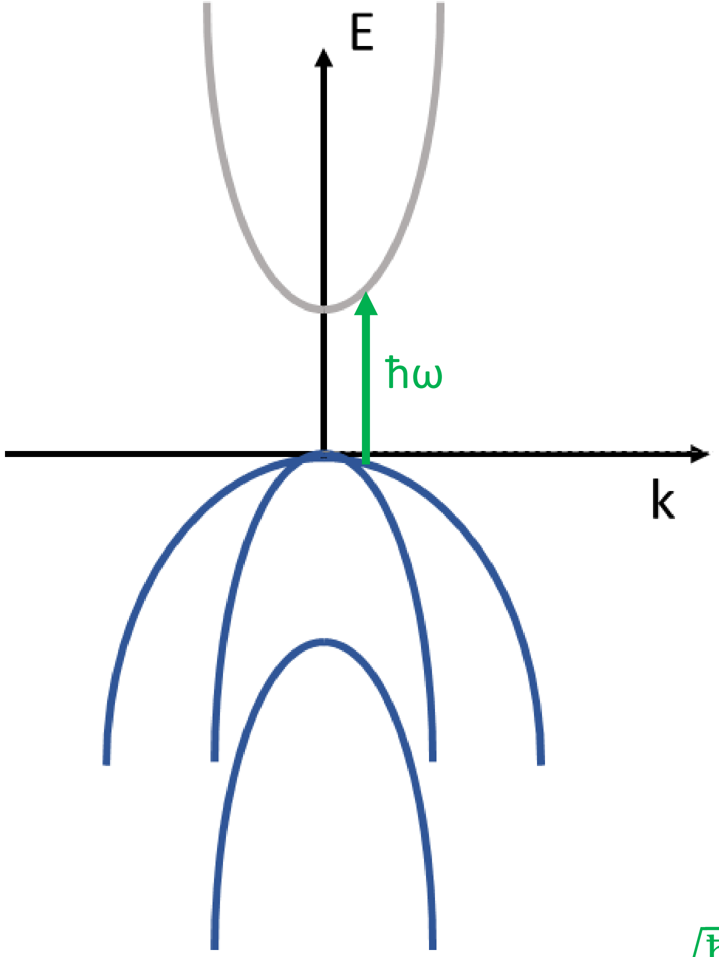
Vertical transitions

Si



Non-vertical transitions

Photon absorption in direct semiconductors



Conservation of Energy

$$E_v = -\frac{\hbar^2 k^2}{2m_h^*}$$

$$E_c = E_g + \frac{\hbar^2 k^2}{2m_e^*}$$

$$\hbar\omega = E_g + \frac{\hbar^2 k^2}{2}\left(\frac{1}{m_e^*} + \frac{1}{m_h^*}\right) = E_g + \frac{\hbar^2 k^2}{2m_r^*}$$

where $\left(\frac{1}{m_e^*} + \frac{1}{m_h^*}\right) = \frac{1}{m_r^*}$

Joint Density of States (density of states available for a transition ħω)

$$D_j(E_{cv}) = 2\int_{S(\tilde{E})} \frac{d^2 S}{(2\pi/L)^3} \frac{1}{|\nabla_{\mathbf{k}} E_{cv}|}$$

Gradient of E_c - E_v in k-space

$$g(\hbar\omega) \propto \frac{\sqrt{\hbar\omega - E_g}}{\hbar\omega}$$

From DOS

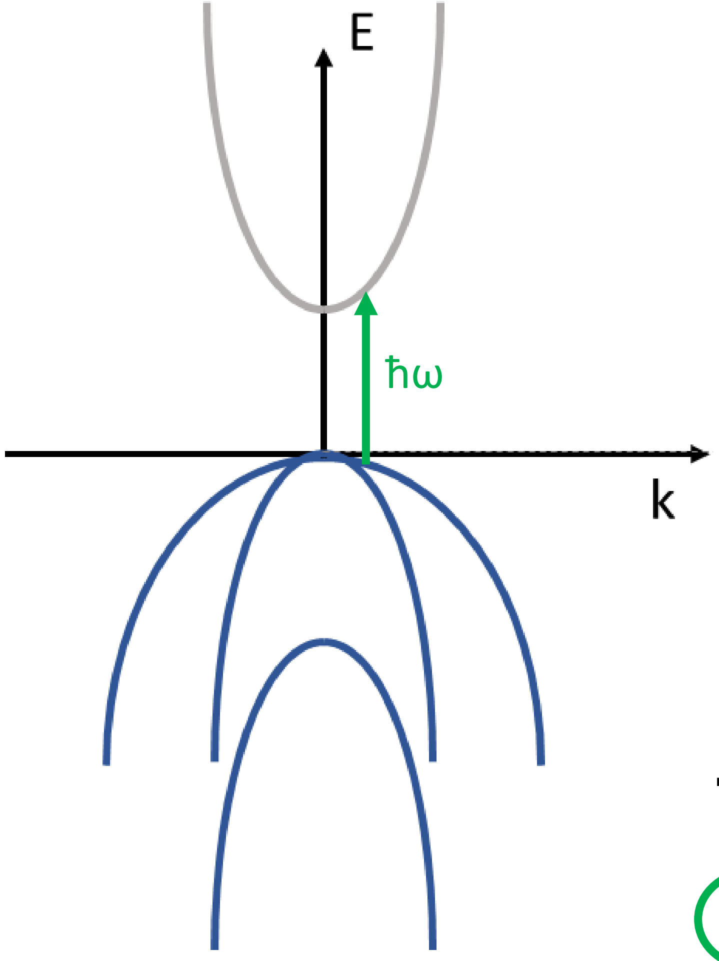
The density of k states can be expressed as a quarter-spherical relation, including the spin-degeneracy:

$$g(k)dk = 2 * \frac{1}{8} * \frac{V}{\pi^3} * 4 * \pi k^2\, dk$$

Spin-degeneracy; Volume of a single state; Volume of a slice of sphere in k-space

$g(E) \propto \sqrt{E}$

Photon absorption in direct semiconductors



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Gradient of E_c - E_v in k-space

Transition rate (~ absorption coefficient)

$$W_{fi} = \frac{2\pi}{\hbar}|M|^2 g(\hbar\omega)\delta(E_C - EV - \hbar\omega)$$

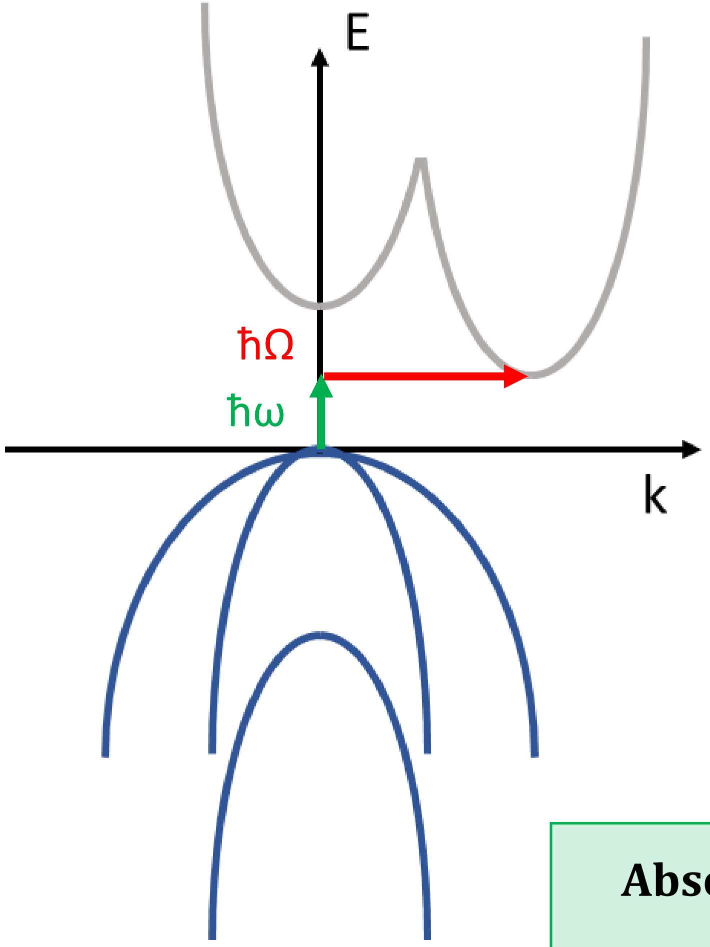
Rate of transitions from an initial state (ψ_i) to a final state (ψ_f)

QM matrix to account for the symmetry of the system (=1 for bulk)

Absorption coefficient

$$\alpha(\hbar\omega) \propto \frac{\sqrt{\hbar\omega - E_g}}{\hbar\omega}$$

Photon absorption in indirect semiconductors



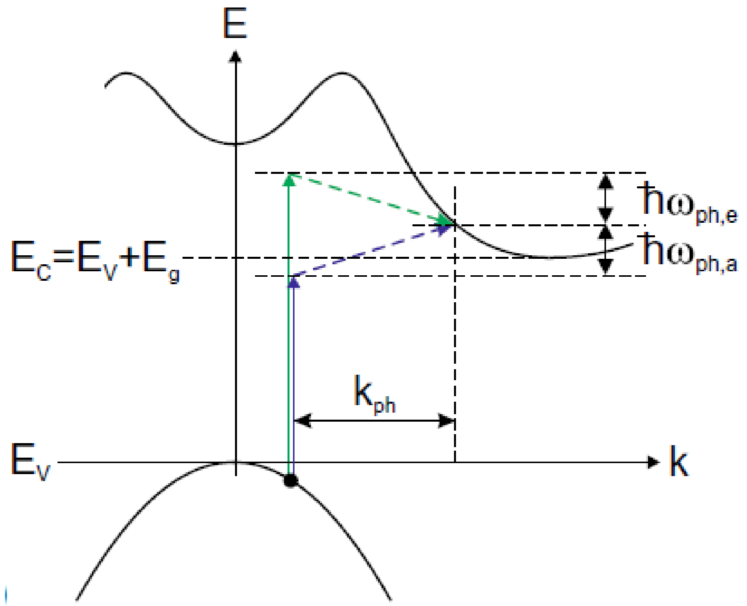
3- particle interaction (electron, photon, phonon)

Due to the increasing complexity of the interaction, the transition rate is expected to be lower than in the case of direct semiconductors.

Conservation of Energy

$$\hbar\omega = E_g + \frac{\hbar^2 k^2}{2m_r^*} \underbrace{\pm \hbar\Omega}$$

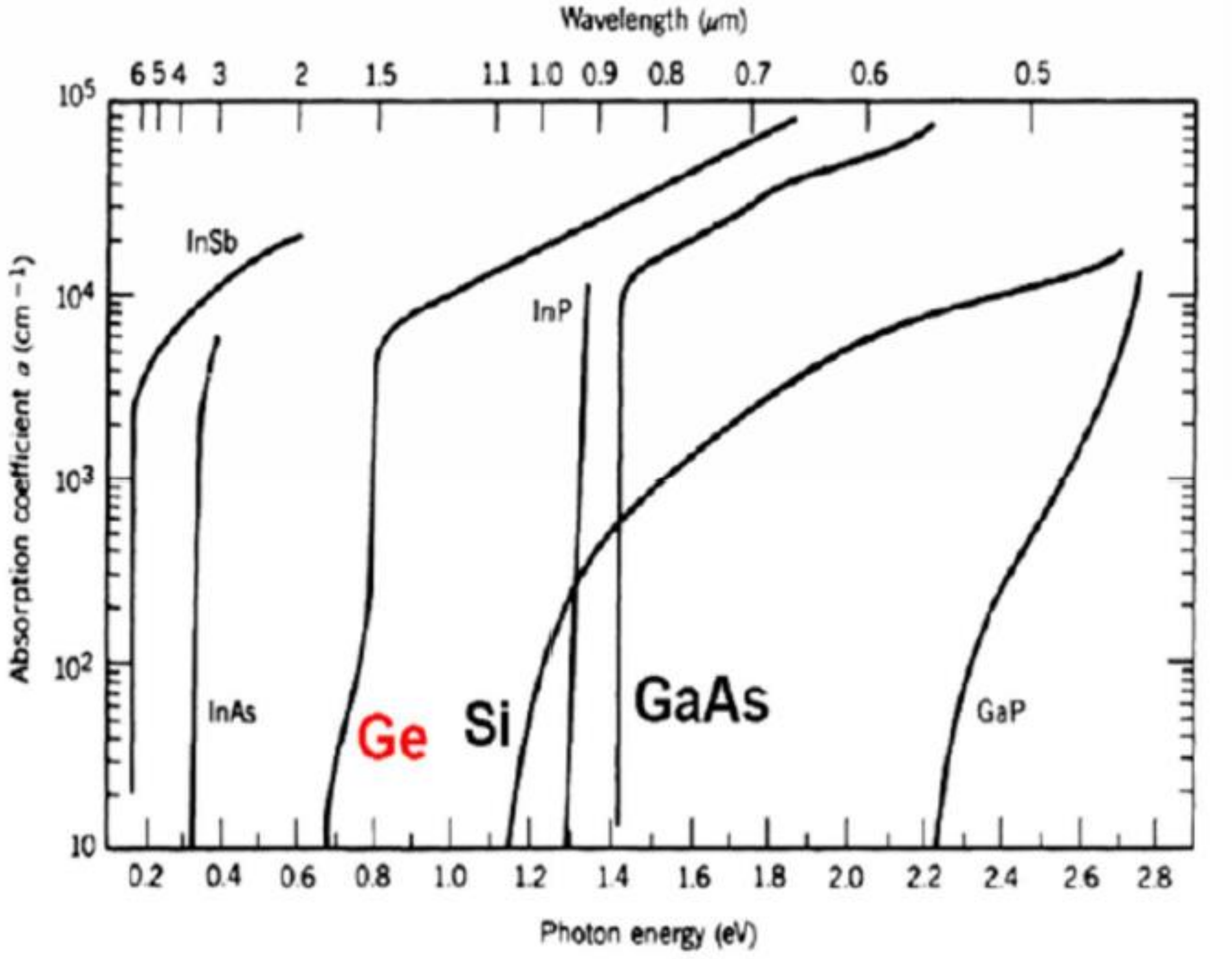
The interaction with phonons allows energy exchange from/to the charge



Absorption coefficient

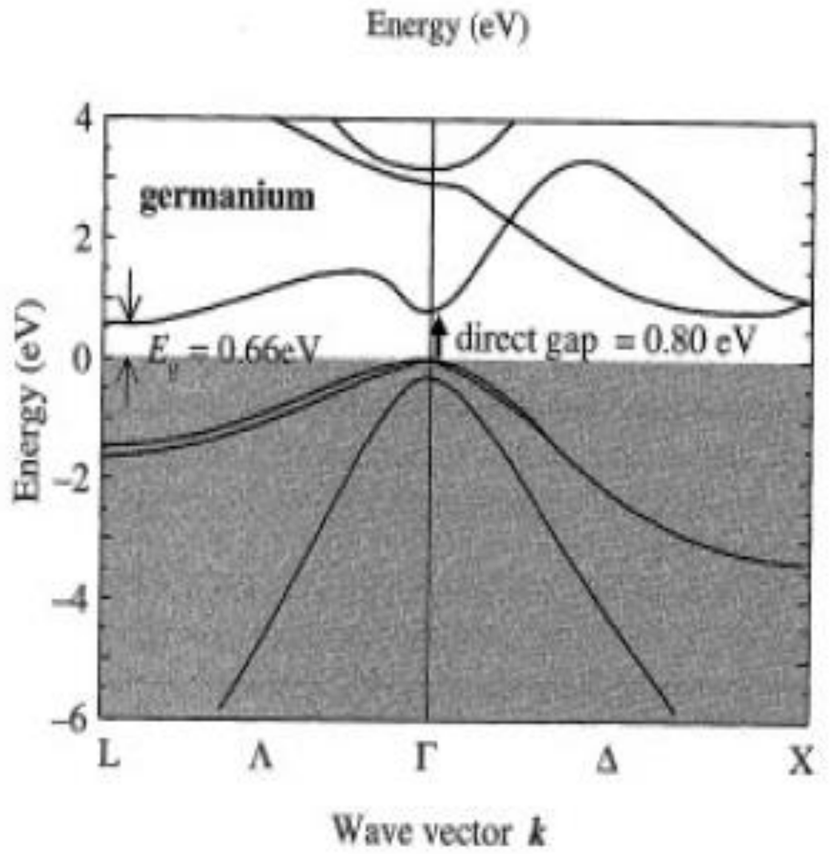
$$\alpha(\hbar\omega) \propto \frac{\left(E_g - \hbar\omega \pm \hbar\Omega\right)^2}{\hbar\omega}$$

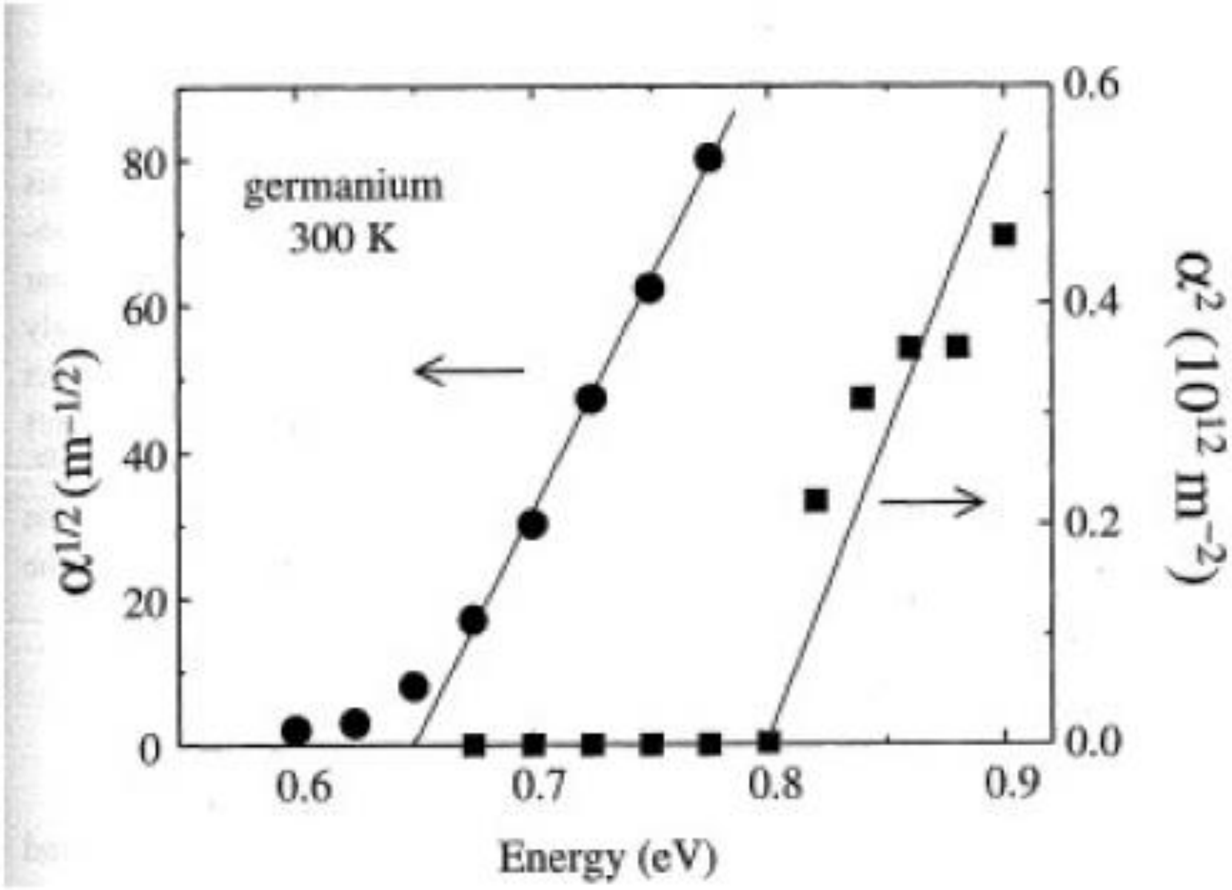
Absorption coefficient of real crystals



Question:
Can you identify the direct semiconductors in the plot?
If so, how?

Absorption coefficient of Ge





Urbach Tail

$$\alpha(E) \propto \exp\left(\frac{E - E_g}{E_0}\right)$$

Urbach Tail

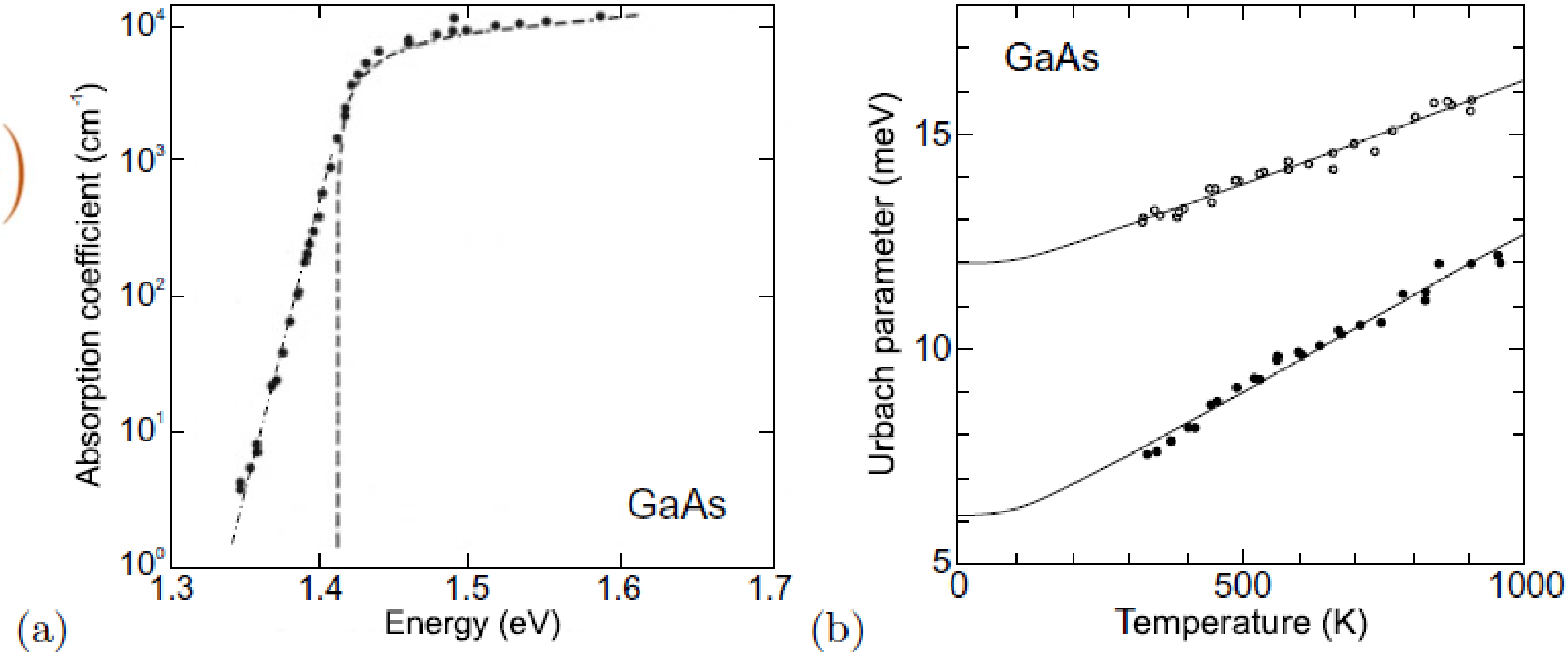
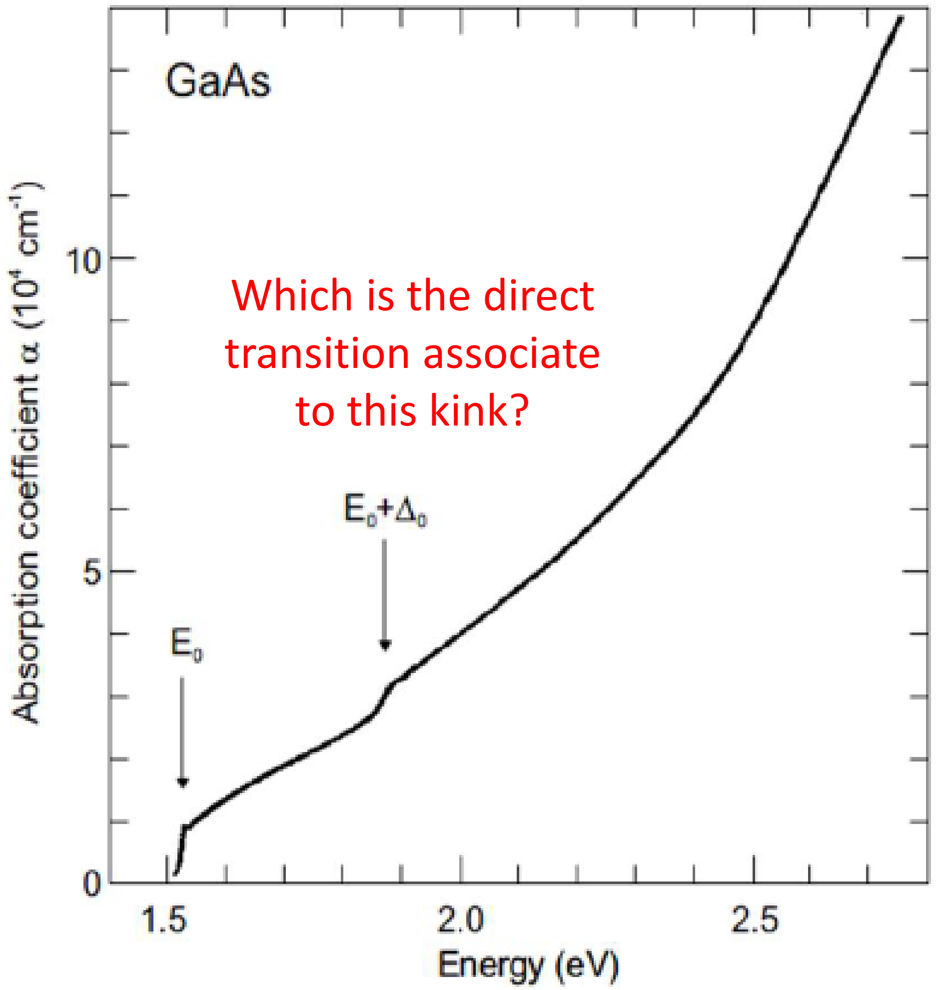
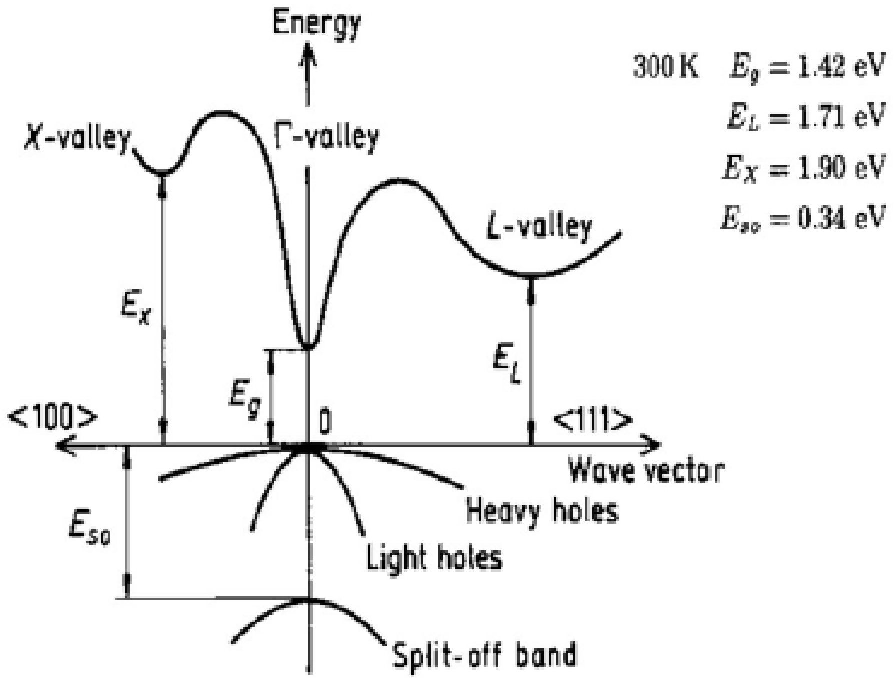


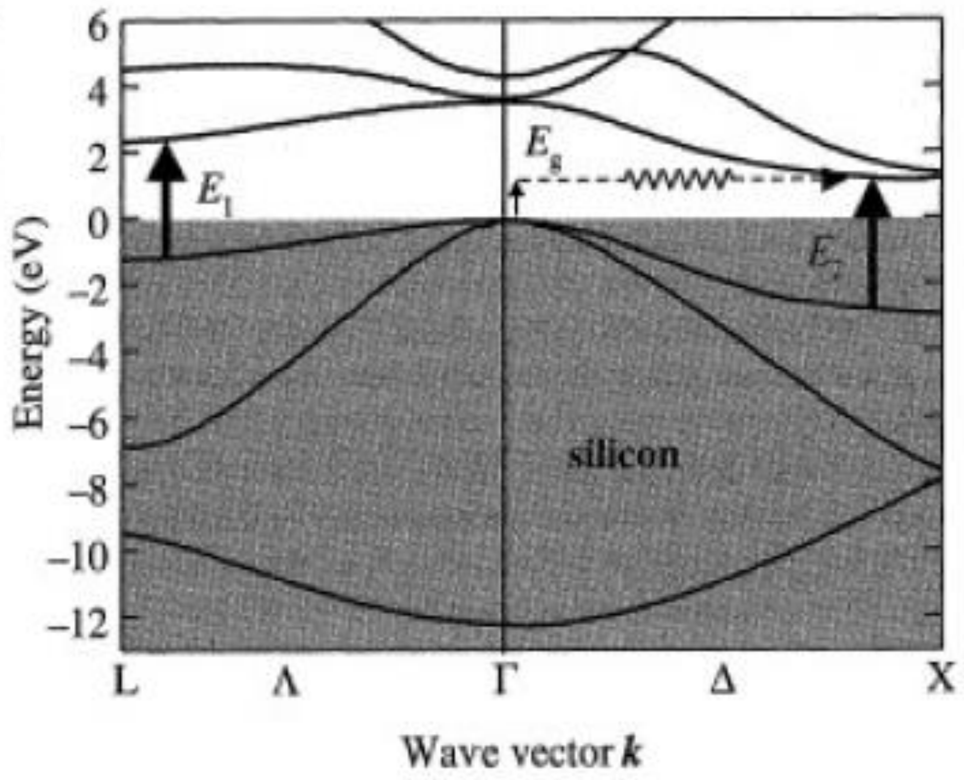
Fig. 9.17 **a** Experimental absorption spectrum (*circles*) of GaAs at room temperature on a semilogarithmic plot. The exponential tail below the band gap is called the Urbach tail (the *dash-dotted* line corresponds to $E_0 = 10.3\,\text{meV}$ in (9.48)). The *dashed line* is the theoretical dependence from (9.45). Adapted from [856]. **b** Temperature dependence of Urbach parameter E_0 for two GaAs samples. Experimental data for undoped (*solid circles*) and Si-doped ($n = 2 \times 10^{18}\,\text{cm}^{-3}$, *empty circles*) GaAs and theoretical fits (*solid lines*) with one-phonon model. Adapted from [854]

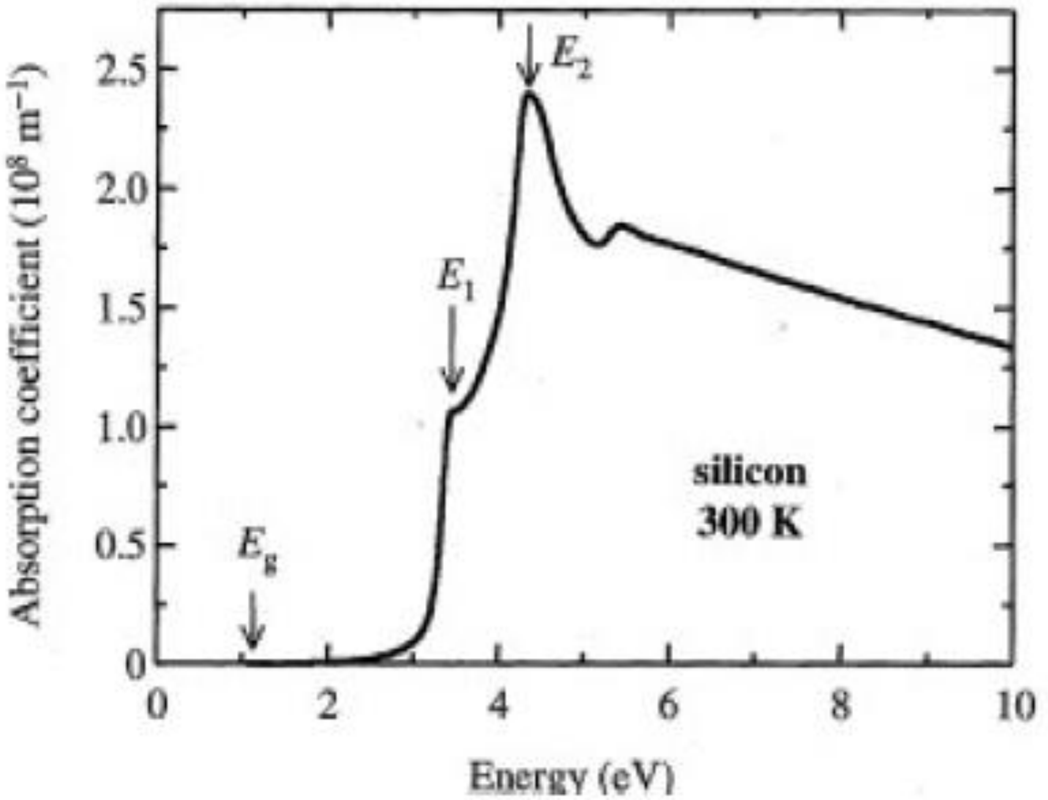
Absorption at higher photon energies



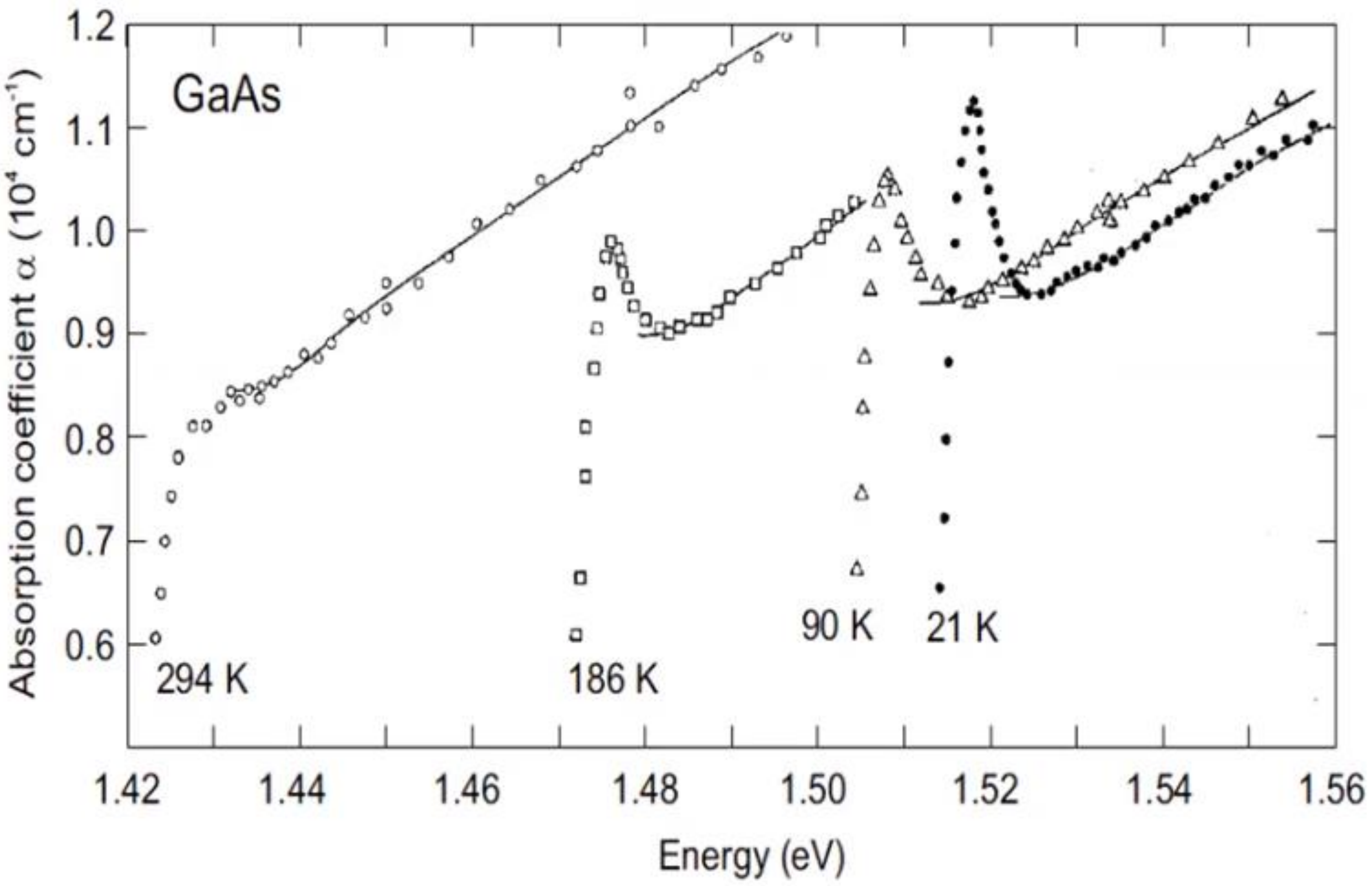


Direct vs indirect transitions in indirect semiconductors

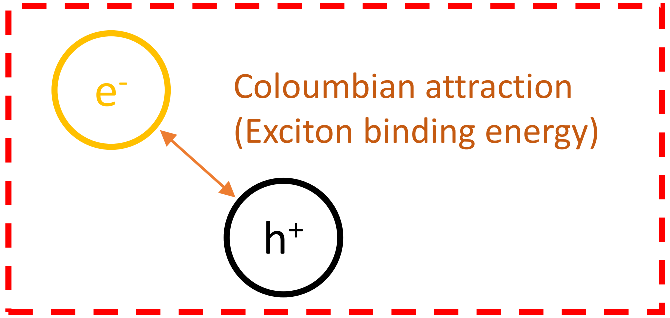




Exciton



Exciton (X)

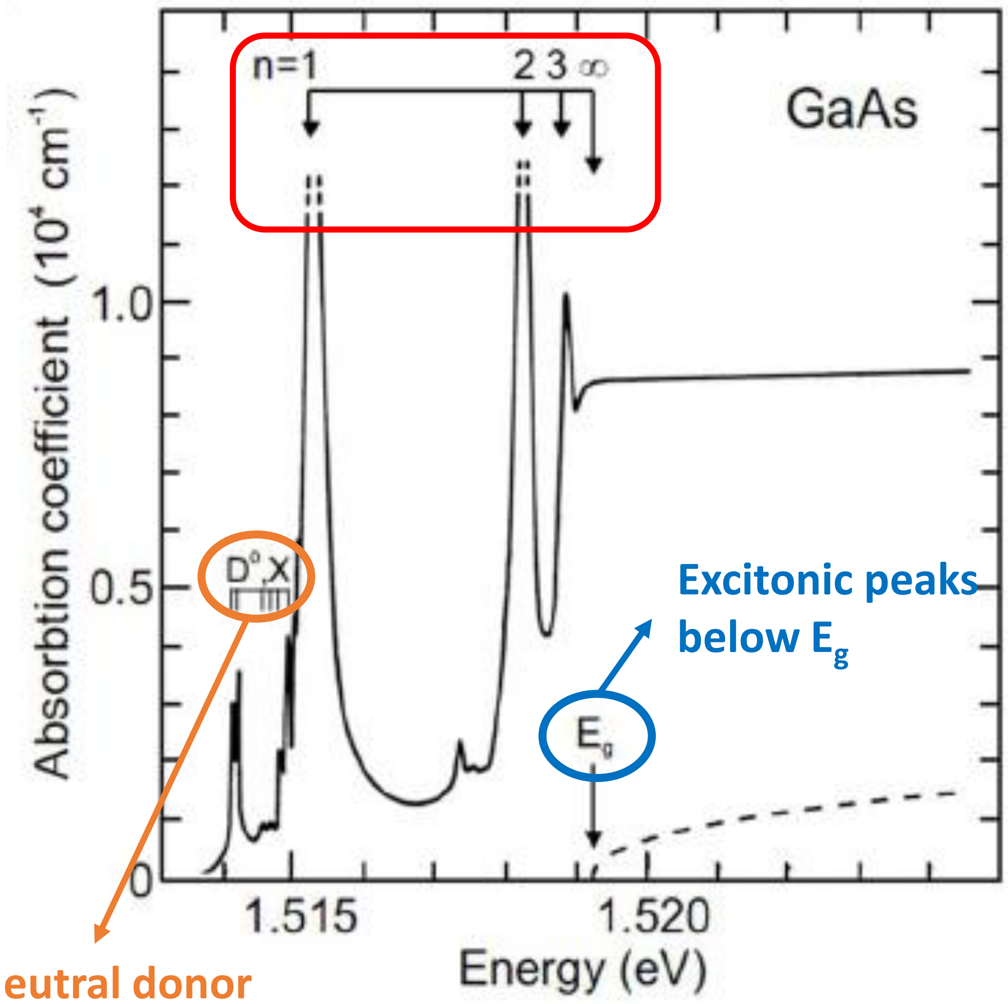


Due to the binding energy, the excitonic peaks lies below the BG

Different excitons can exists depending on their interaction with the surroundings

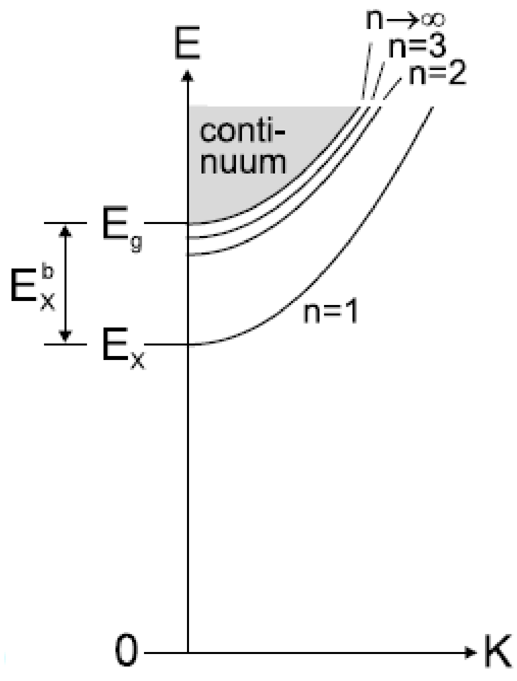
Quantum nature of exciton

Atom-like energetic quantization



Excitonic peaks below E_g

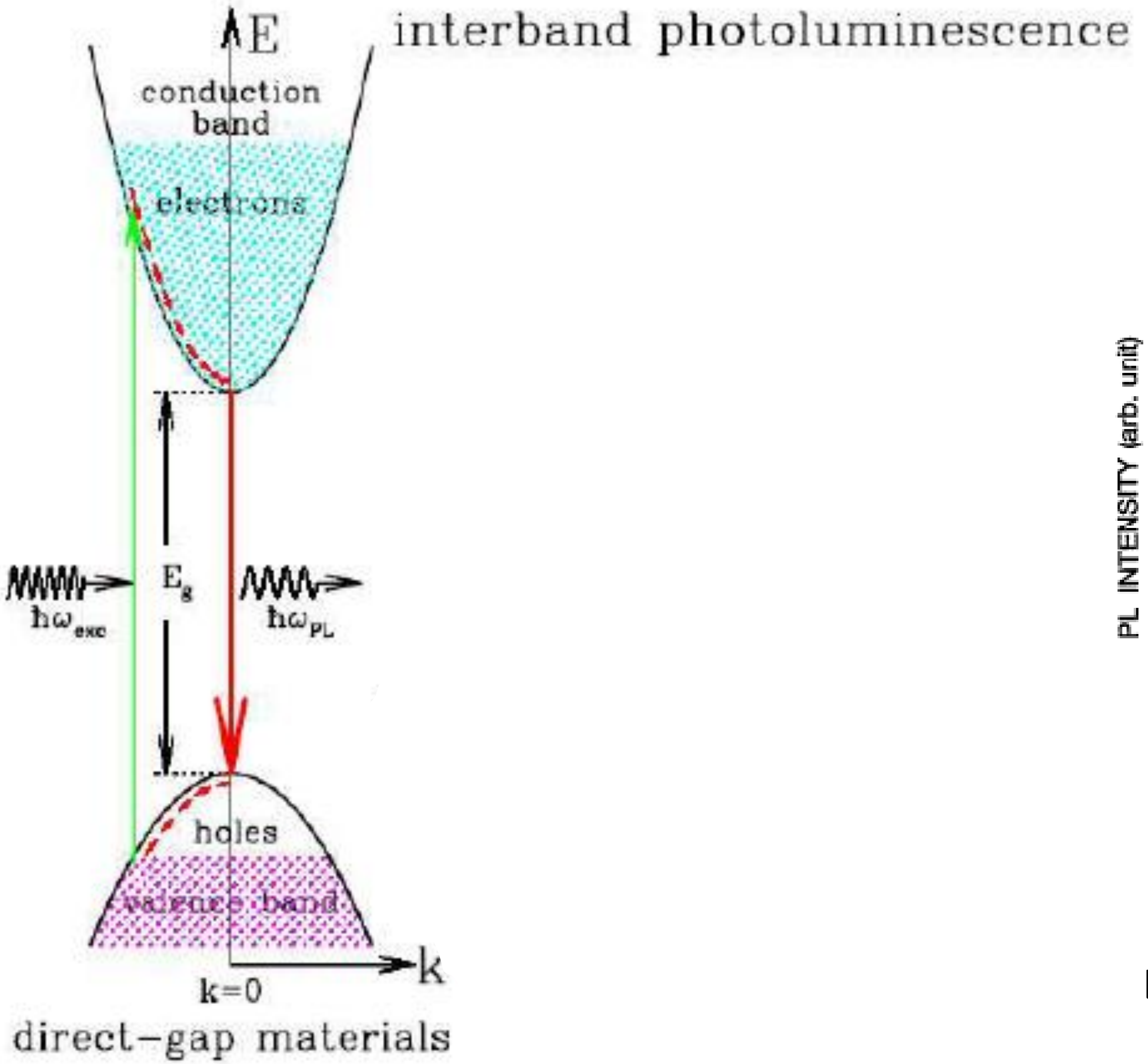
Neutral donor bound exciton

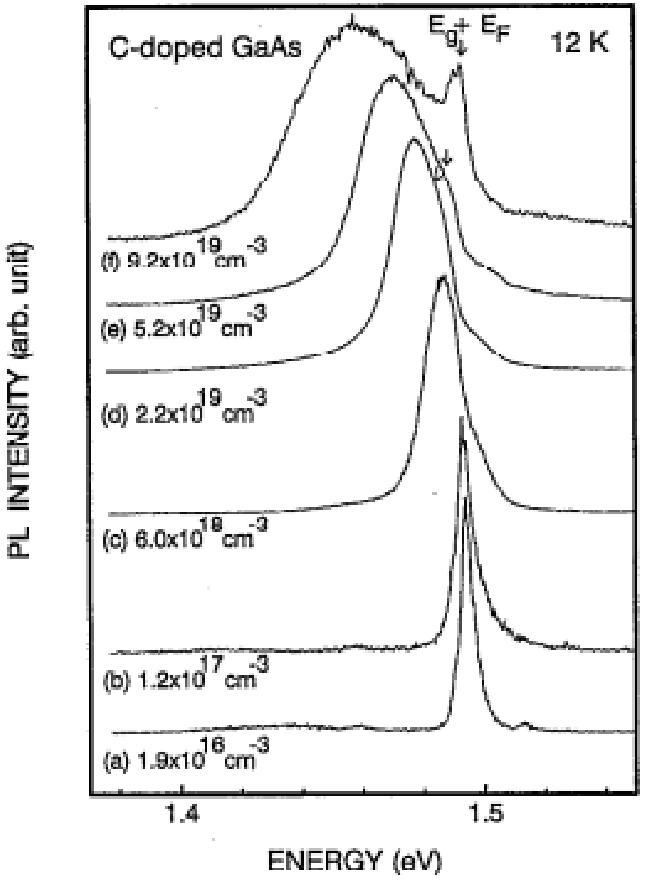


Photoluminescence

Excitation Energy

Emission Energy





Low T PL spectra for doped GaAs