Optical transitions in semiconductors

Semiconductor devices II - EE-567

edoardo.lopriore@epfl.ch

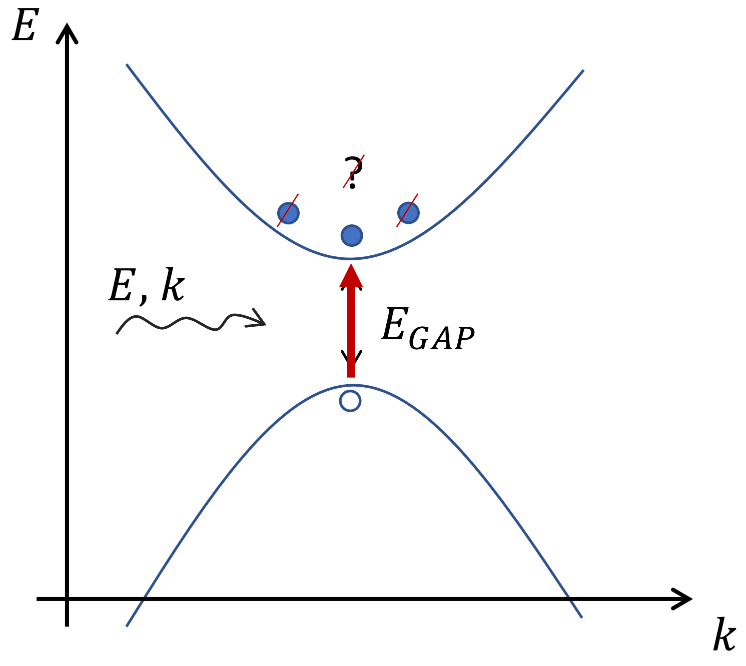
fedele.tagarelli@epfl.ch

K-Selection Rule

- Conversation of momentum is true for semiconductors: Δp = 0;

- Another way to write it : Δk = 0 so $k_0 = k_{final}$;

What this means for **direct bandgap semiconductor**



For optoelectronic devices we are interested in interactions between electrons and photons. Main points:

1. Energetic requirement for radiative interactions: $E > E_{GAP}$

2. Conservation of momentum:

$$k_C = k_V + k_{Ph}$$

$$k_C, k_V = \frac{2\pi}{a} \approx 10^9 - 10^{10} cm^{-1}$$

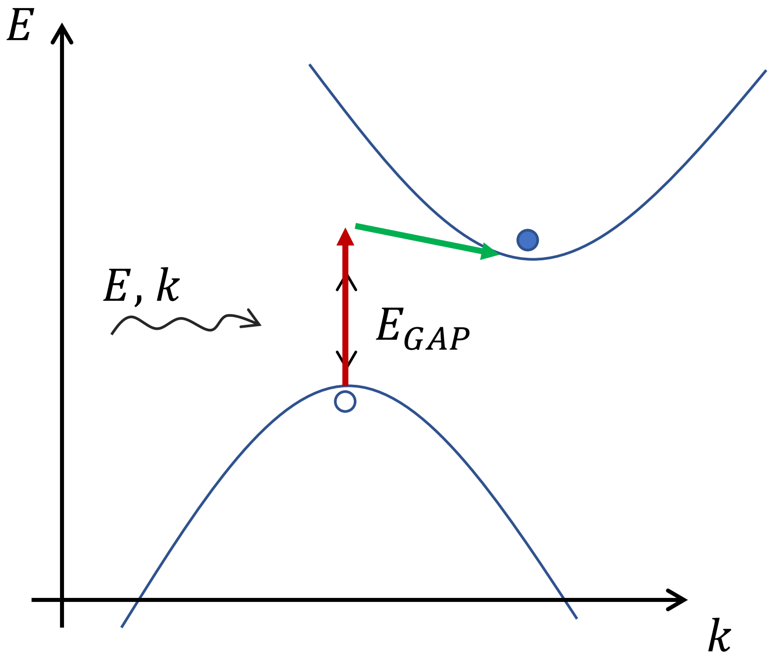
$$k_{Ph} = \frac{2\pi}{\lambda} \approx 10^4 cm^{-1}$$

K-Selection Rule

- Conversation of momentum is true for semiconductors: $\Delta p = 0$;

- Another way to write it : $\Delta k = 0$ in total;

What this means for **in-direct bandgap semiconductor**



For optoelectronic devices we are interested in interactions between electrons and photons. Main points:

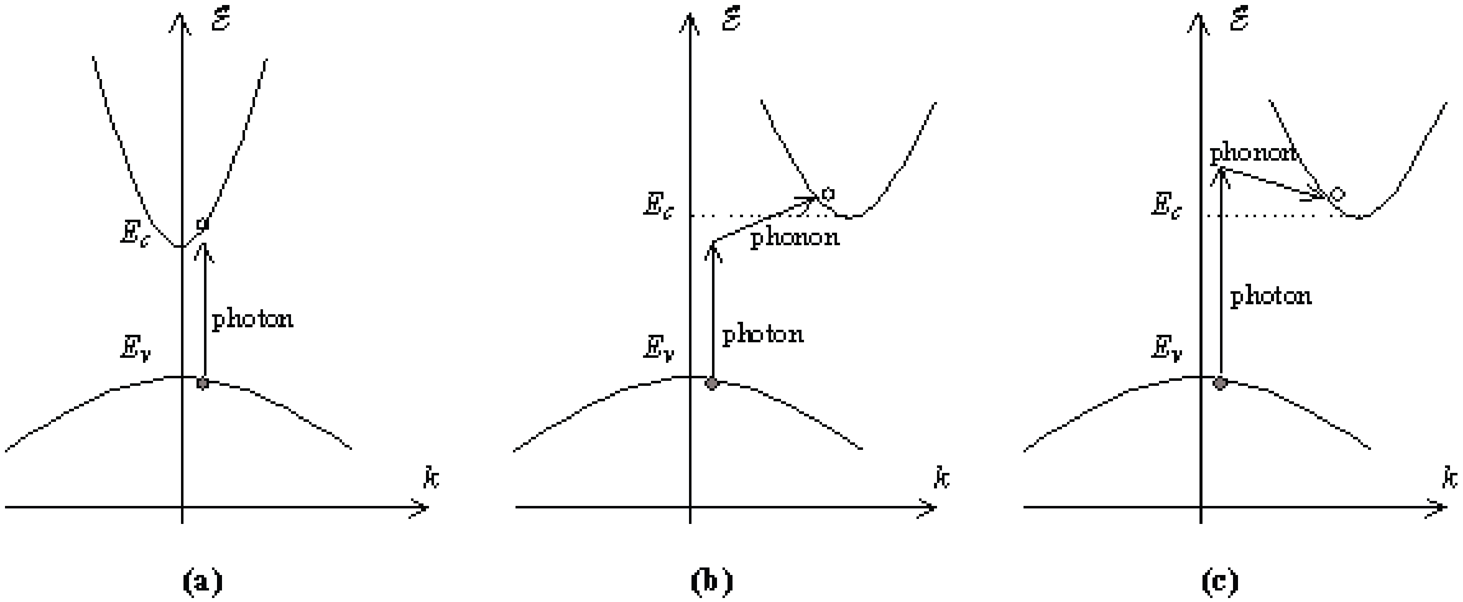
1. Energetic requirement for radiative interactions: $E > E_{GAP}$

2. Conservation of momentum:

$$k_C = k_V + \cancel{k_{Ph}} + k_{Phonon}$$

Phonons have momentum comparable to that of electrons in the lattice

Summary of Optical properties of semiconductors



How to quantify these microscopic phenomena?

Direct Semiconductor

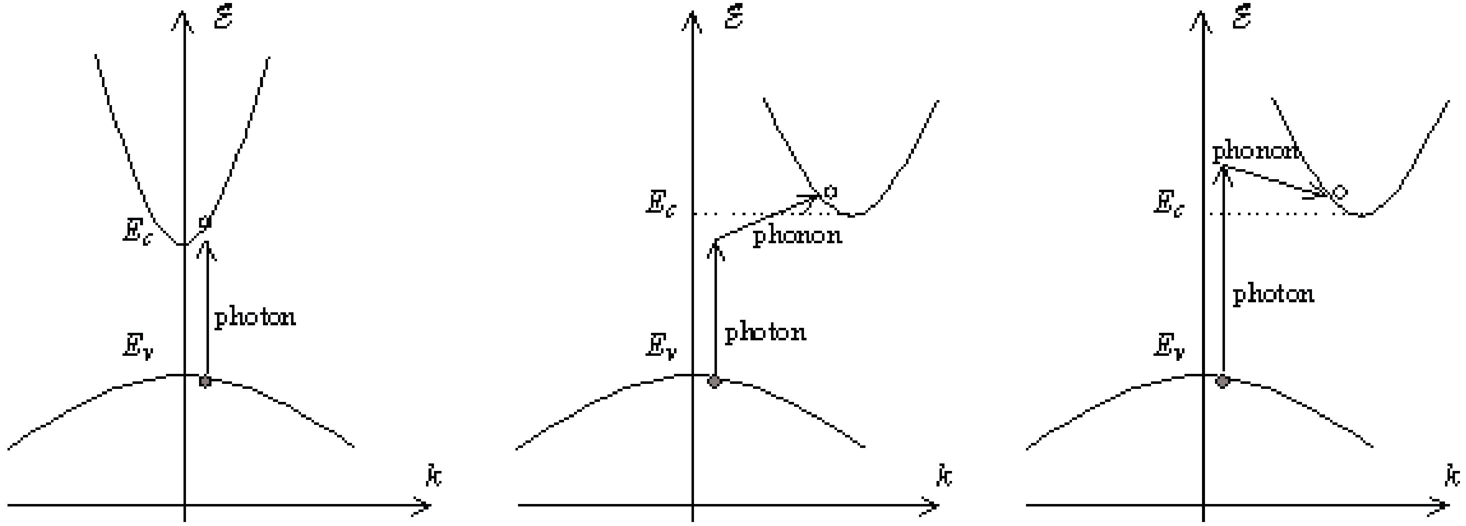
(a) Photon absorption in a direct bandgap semiconductor

Indirect Semiconductor

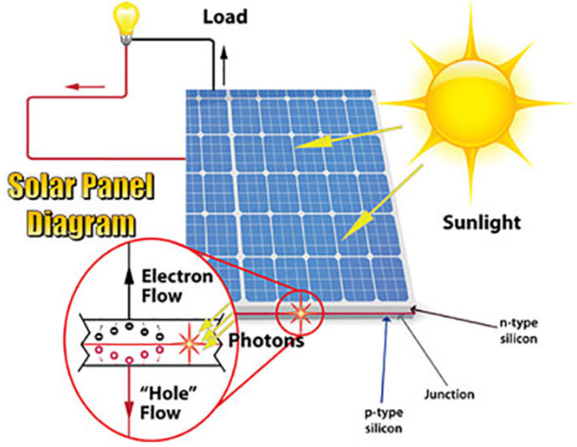
(b) Photon absorption in an indirect bandgap semiconductor assisted by phonon absorption and

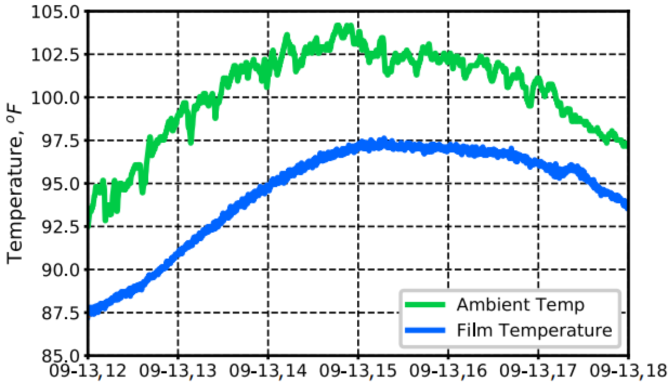
(c) Photon absorption in an indirect bandgap semiconductor assisted by phonon emission.

Applications of Optical properties of semiconductors



(c)





Data measured from rooftop in Mountain View, CA on 9.13.2019

Optical properties of semiconductors

$$H_0 = \frac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{r})$$

In presence of an EM field described by a vector potential $\boldsymbol{A}(\boldsymbol{r}, t)$:

$$H = \frac{1}{2m}\left[\boldsymbol{p} + \frac{e}{c}\boldsymbol{A}(\boldsymbol{r}, t)\right]^2 + V(\boldsymbol{r}) = H_0 + \frac{e}{mc}\boldsymbol{A} \cdot \boldsymbol{p} + \frac{e^2}{2mc^2}\boldsymbol{A}^2$$

Optical properties of semiconductors

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Perturbation Theory

In presence of an EM field described by a vector potential $\boldsymbol{A}(\boldsymbol{r}, t)$:

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From the Lagrangian of a charged particle in a EM field, derived directly from Maxwells' equations

$$L = \frac{1}{2}\, m\, \boldsymbol{v}\cdot\boldsymbol{v} + eV + \frac{e}{c}\, \boldsymbol{v}\cdot\boldsymbol{A} \longrightarrow p_{tot} = \frac{\partial L}{\partial v} = p + \frac{e}{c}A$$

Optical properties of semiconductors

$$H_0 = \frac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{r})$$

In presence of an EM field described by a vector potential $\boldsymbol{A}(\boldsymbol{r}, t)$:

The field is not extremely strong and e^2 is small, thus this term can be neglected

$$H = \frac{1}{2m}\left[\boldsymbol{p} + \frac{e}{c}\boldsymbol{A}(\boldsymbol{r}, t)\right]^2 + V(\boldsymbol{r}) = H_0 + \frac{e}{mc}\boldsymbol{A}\cdot\boldsymbol{p} + \frac{e^2}{2mc^2}\boldsymbol{A}^2$$

For example $\boldsymbol{A}(r, t) = A_0\hat{\boldsymbol{e}}e^{i(\boldsymbol{q}\cdot\boldsymbol{r}-\omega t)} + c.c.$ with $\hat{\boldsymbol{e}} \perp \boldsymbol{q}$

$$H = H_0 + \frac{eA_0}{mc}e^{i(\boldsymbol{q}\cdot\boldsymbol{r}-\omega t)}\hat{\boldsymbol{e}}\cdot\boldsymbol{p} + \frac{eA_0}{mc}e^{-i(\boldsymbol{q}\cdot\boldsymbol{r}-\omega t)}\hat{\boldsymbol{e}}\cdot\boldsymbol{p}$$

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Absorbed photon Emitted photon

Fermi golden rule

Coupling between initial and final states

Density of states in the transition

$$W_{ij} = \frac{2\pi}{\hbar} |\langle i|H'|j\rangle|^2 \rho(E_f)$$

W_{ij} is the *transition probability per unit time* between two quantum states i, j

$\rho(E_f)$ is the density of final states. If energy is conserved: $\rho(E_f) = \delta(E)$

H' is the perturbation term in the Hamiltonian

$|\langle i|H'|j\rangle|$ is the matrix element for the interaction

In our case:

$$W_{i\to j} = \frac{2\pi}{\hbar}\left(\frac{eA_0}{mc}\right)^2 \left|\langle \psi_j|e^{i\boldsymbol{q}\cdot\boldsymbol{r}}\hat{\boldsymbol{e}}\cdot\boldsymbol{p}|\psi_i\rangle\right|^2 \delta(E_j - E_i - \hbar\omega)$$

$$W_{j\to i} = \frac{2\pi}{\hbar}\left(\frac{eA_0}{mc}\right)^2 \left|\langle \psi_i|e^{-i\boldsymbol{q}\cdot\boldsymbol{r}}\hat{\boldsymbol{e}}\cdot\boldsymbol{p}|\psi_j\rangle\right|^2 \delta(E_i - E_j + \hbar\omega)$$

Absorbed photon
$E_j = E_i + \hbar\omega$

Emitted photon
$E_i = E_j - \hbar\omega$

Transitions

We have many i,j states from and to which the the transition can happen

The net transition rate from i to j is given by $W_{ij} - W_{ji}$. Over all states:

$$W = \sum_{ij} W_{ij} - W_{ji}$$

← Considering photons interacting with a semiconductor, it represents the net absorption rate

Every state has an occupation probability given by $f(E)$

To have a transition between i and j, we need occupied i and empty j: $f(E_i)[1 - f(E_j)]$

So, we multiply W_{ij} by $f(E_i)[1 - f(E_j)]$ and W_{ji} by $f(E_j)[1 - f(E_i)]$:

$$W = \frac{2\pi}{\hbar}\left(\frac{eA_0}{mc}\right)^2 2\sum_{ij}\left|\langle\psi_j|e^{i\boldsymbol{q}\cdot\boldsymbol{r}}\hat{\boldsymbol{e}}\cdot\boldsymbol{p}|\psi_i\rangle\right|^2 \delta(E_j - E_i - \hbar\omega)\,[f(E_i) - f(E_j)]$$

Transitions

$$W = \frac{2\pi}{\hbar}\left(\frac{eA_0}{mc}\right)^2 2\sum_{ij}\left|\langle\psi_j|e^{i\boldsymbol{q}\cdot\boldsymbol{r}}\hat{\boldsymbol{e}}\cdot\boldsymbol{p}|\psi_i\rangle\right|^2\delta(E_j - E_i - \hbar\omega)\,\underbrace{[f(E_i) - f(E_j)]}_{=1 \text{ at } T=0}$$

In the limit for T = 0, full VB and empty CB:

$$W \sim \sum_{\text{occ. } i}\sum_{\text{free } j}\left|\langle\psi_j|e^{i\boldsymbol{q}\cdot\boldsymbol{r}}\hat{\boldsymbol{e}}\cdot\boldsymbol{p}|\psi_i\rangle\right|^2\delta(E_j - E_i - \hbar\omega)$$

$$\sim \sum_{cv}\int_{BZ}|\hat{\boldsymbol{e}}\cdot\langle\psi_{c\boldsymbol{k}}|\boldsymbol{p}|\psi_{v\boldsymbol{k}}\rangle|^2\delta(E_{c\boldsymbol{k}} - E_{v\boldsymbol{k}} - \hbar\omega)\frac{d\boldsymbol{k}}{(2\pi)^3}$$

Perturbation theory → we can apply our knowledge on the wavefunctions in the case without perturbations and solve the calculation of the net absorption rate

Joint density of states

The dipole matrix elements are smooth functions of the k-vector.
Thus, they do not affect much the integral, and can be factorized out.

On the contrary, the main term to determine the behaviour of the calculation is $\delta(E_{c\boldsymbol{k}} - E_{v\boldsymbol{k}} - \hbar\omega)$

Essentially, the integral is controlled by the so-called *joint density of states*:

$$\rho_{cv}(\omega) = \int \delta(E_{c\boldsymbol{k}} - E_{v\boldsymbol{k}} - \hbar\omega)\frac{d\boldsymbol{k}}{(2\pi)^3} \quad \rightarrow \quad \rho_{cv}(\omega)^{3D} = 2\pi\left(\frac{2m^*}{\hbar^2}\right)^{\frac{3}{2}}\sqrt{\hbar\omega - E_g}$$

Specific case of a **direct** bandgap semiconductor in **3D**

Dielectric function and transition rate

The *total energy per unit time* dissipated in the system (volume V) is:

$$P(q,\omega) = \hbar\omega W(q,\omega)$$

From Maxwell equations we know that

$$\left.\begin{aligned}&\frac{\partial D}{\partial t} = \frac{\partial E}{\partial t} + 4\pi J\\ &D = \epsilon_1 + i\epsilon_2\\ &J = \sigma \cdot E\end{aligned}\right\} \longrightarrow \epsilon = 1 + \frac{4\pi i\sigma}{\omega}$$

$$\hbar\omega W = \frac{\omega}{4\pi i}(\epsilon - 1)|E_0|^2 V$$

Also, from general electromagnetism:

$$P = \int_V J \cdot E\, dr = \int_V \sigma E \cdot E\, dr = \sigma |E_0|^2 V$$

Thus we connect the microscopic description to the macroscopic quantities σ, ϵ

Absorption coefficient

In the end we find:

$$\epsilon_2(\boldsymbol{q},\omega) = \frac{2\pi\hbar c^2}{\omega^2}\frac{1}{V}\frac{W(\boldsymbol{q},\omega)}{A_0^2}$$

$$\alpha(\omega) = \frac{2\pi\hbar c}{n(\omega)\omega}\frac{1}{V}\frac{W(\omega)}{A_0^2}$$

$$I(z) = I_0 e^{-\alpha(\omega)z}$$

Familiar **macroscopic** absorption law

Absorption coefficient

Direct Bandgap in 3D:

$$\alpha \approx \sqrt{hv - E_G}$$

Indirect Bandgap:

$$\alpha \propto \frac{(hv - E_G - E_P)^2}{e^{\frac{E_p}{kT}} - 1} - \frac{(hv - E_G - E_P)^2}{1 - e^{-\frac{E_p}{kT}}}$$

Direct Bandgap is more efficient for photon absorption: MoS_2, GaAs, InP…