Optics of semiconductor nanostructures: an overview

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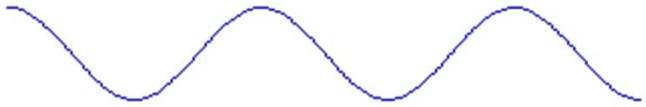
“One should not work on semiconductors, that is a filthy mess; who knows whether they really exist.”

Wofgang Pauli 1931

Lecture 1

Electron states and optical properties of bulk semiconductors and quantum wells



Free particle can have any energy

Confined particle has a discrete set of possible states and discrete set of energies.

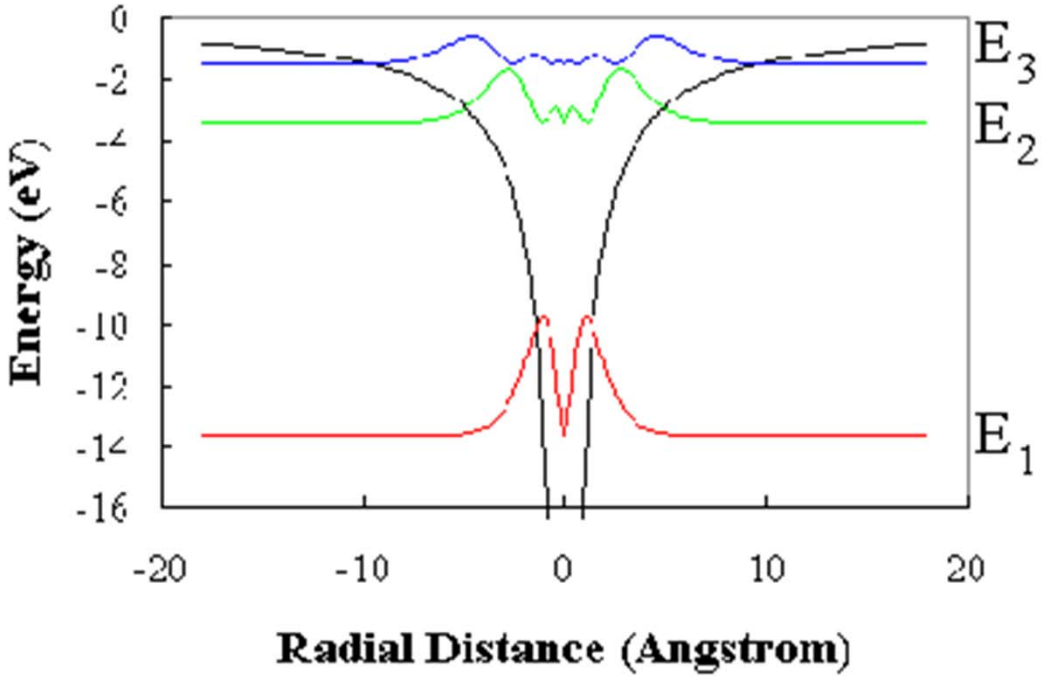
These states determine all optical properties.

Electrons in atoms are confined, but only a bunch of different atoms exist, with rigid selection rules

Electrons in crystals: only band-to-band transitions, with rigid constraints due to crystal symmetry and selection rules

By confining electrons in nanostructures, one can create “artificial atoms” with any optical property on demand

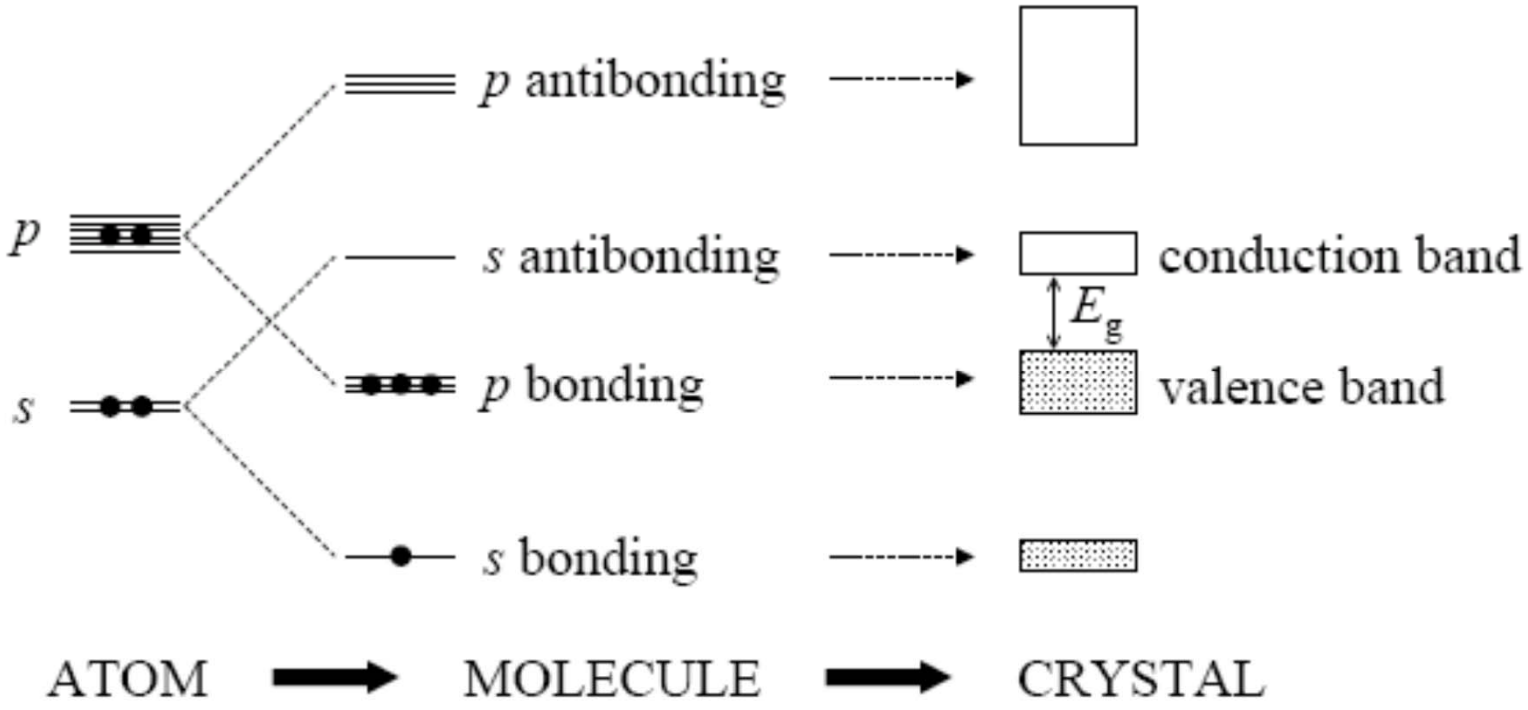
The hydrogen atom potential and wavefunction



Optical transitions are determined by properties of atoms (confining potential, symmetry, etc.)

Band formation from overlapping atomic orbitals

Now bring atoms together (to a distance of 3 A from each other)



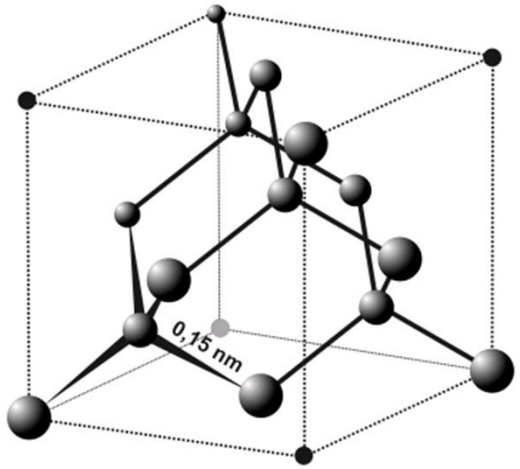
Electron states in crystals

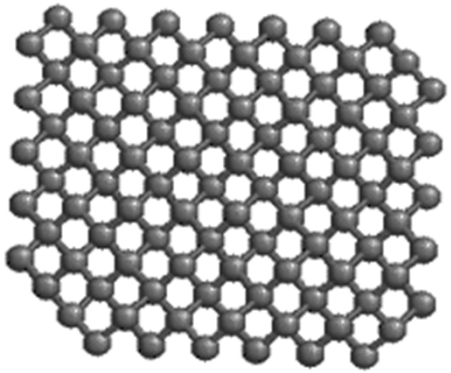
Dense many-body quantum systems: 10^{22} particles per cm^3

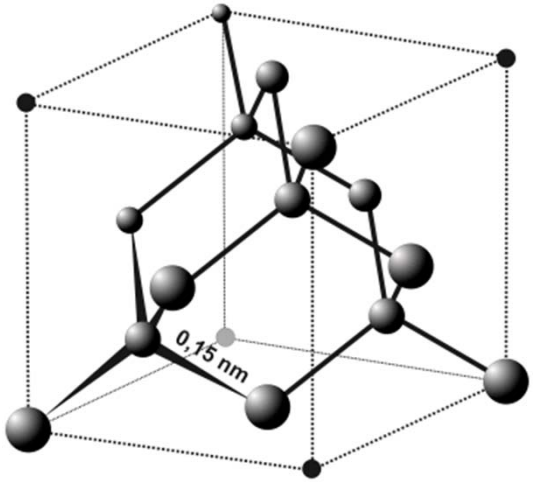
It seems to be hopeless to find wave functions and energy spectra

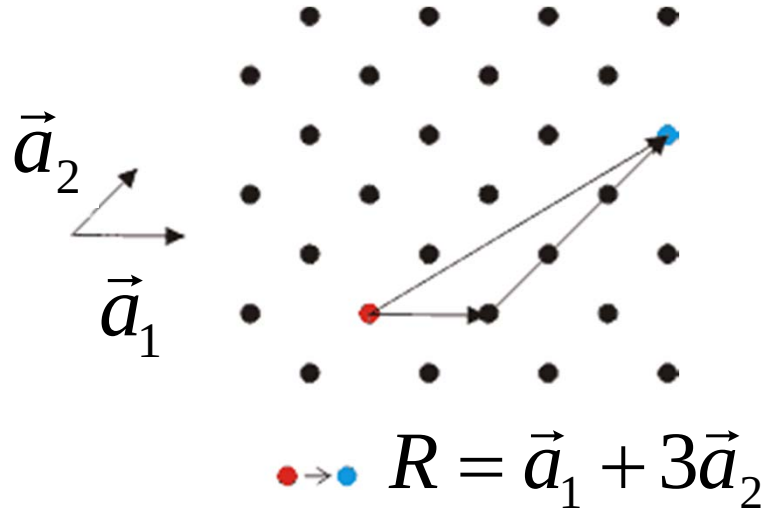
However, crystal lattice symmetry helps tremendously

Crystal potential consists of a 3D lattice of ionic core potentials screened by the inner shell electrons, which are further surrounded by the bond charge distributions which hold everything together









A unit lattice cell is spanned by primitive vectors $\vec{a}_i$

The whole lattice is spanned by their linear combination:

$$\vec{R}_n = \sum_i n_i \vec{a}_i$$

1) **Replace a many-body problem of interacting electrons and ions with motion of a single "electron" in the effective potential created by all other particles;**

2) **Assume that the effective crystal potential has the symmetry and periodicity of a lattice**

Schroedinger's equation for a single electron in a periodic potential *V*(r):

$$\left\{\frac{p^2}{2m_0}+V(\mathbf{r})+\frac{\hbar}{4m_0^2c^2}[\nabla V\times\mathbf{p}]\cdot\sigma\right\}\psi \;=\; E\psi,$$

Introduce translation operator

$$T_n\psi(k,r)=\psi(k,r+R_n)=t_n\psi(k,r)$$

$\psi(k,r)$ **is eigen function of both *H* and T_n ; *k* is the quantum number associated with T_n.**

t_n is a phase factor with $|t_n| = 1$ $\quad \psi(k,r+R_n)=e^{ikR_n}\psi(k,r)$

Bloch theorem:

$$\psi_\lambda=\frac{1}{L^{3/2}}e^{ikr}u_\lambda(k,r)$$ **- Bloch functions**

$$u_\lambda(k,r)=u_\lambda(k,r+R_n)$$

A simpler argument:

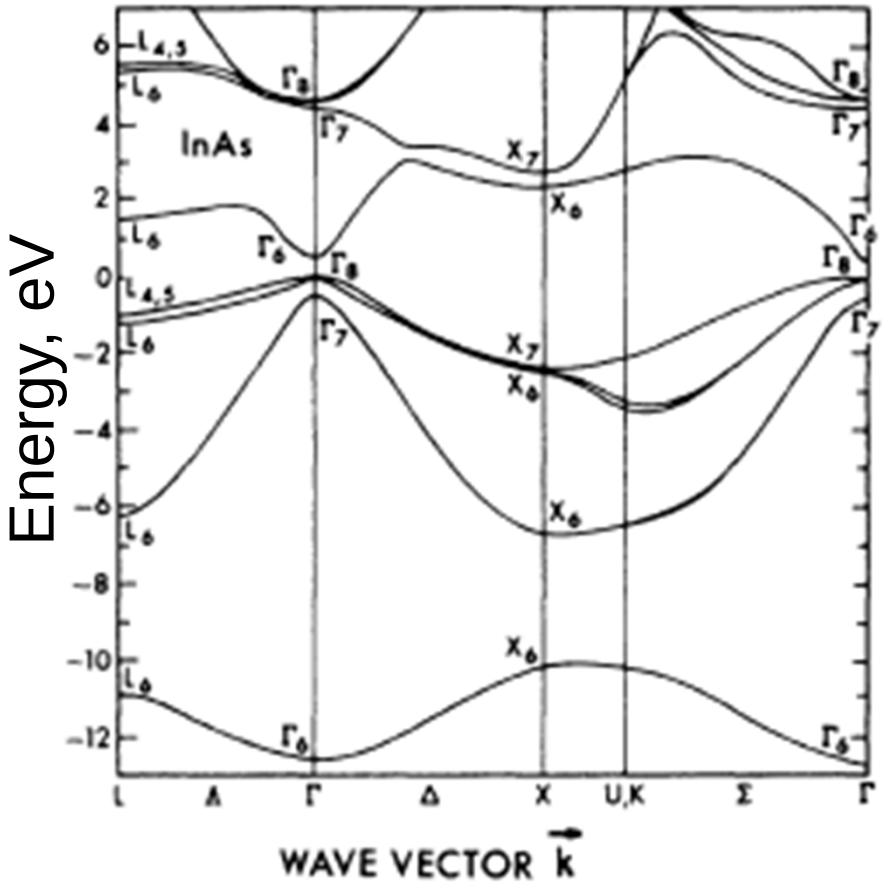
$$V(r+R_n)=V(r)$$

$$|\psi(r+R_n)|^2=|\psi(r)|^2$$

$$\psi(k,r+R_n)=e^{ikR_n}\psi(k,r)$$

Bloch theorem: $\psi_\lambda=\frac{1}{L^{3/2}}e^{ikr}u_\lambda(k,r)$

For each k, there is a set of energies $E_\lambda(k)$.
With changing k, they form continuous *bands,* separated by forbidden bands, or band gaps.



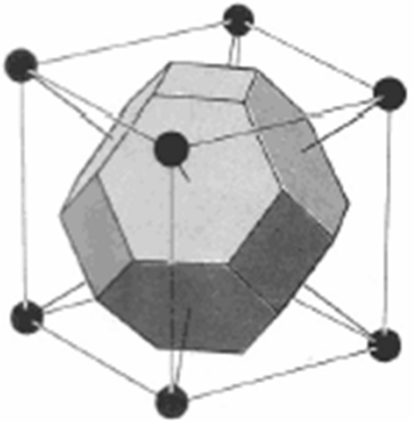
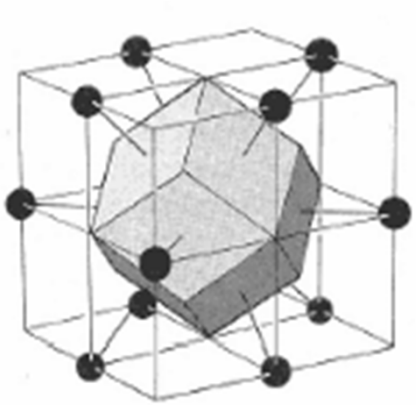
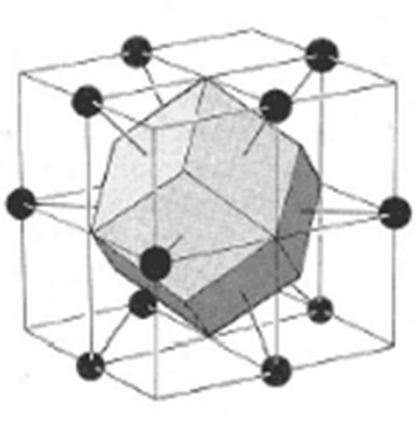
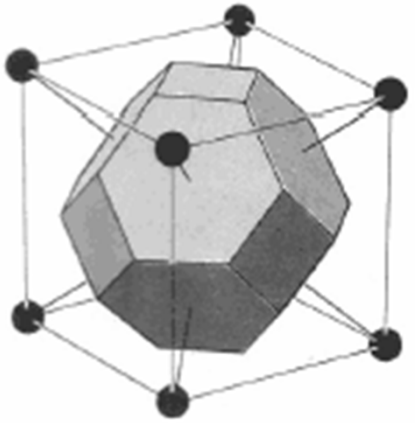
Bands are periodic in k:
E(k+g) = E(k)
g – the vector of reciprocal lattice

$$V(r) = \sum_g C(g) e^{igr}$$

g should satisfy $e^{igR_n} = 1$

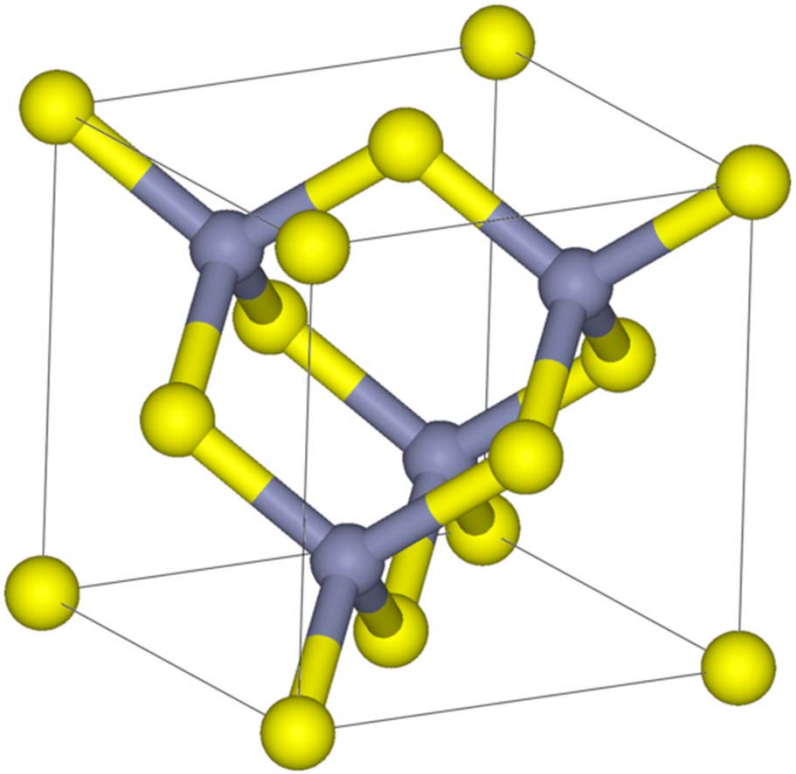
$$g = \sum_i n_i b_i ; b_i a_j = 2\pi\delta_{ij}$$

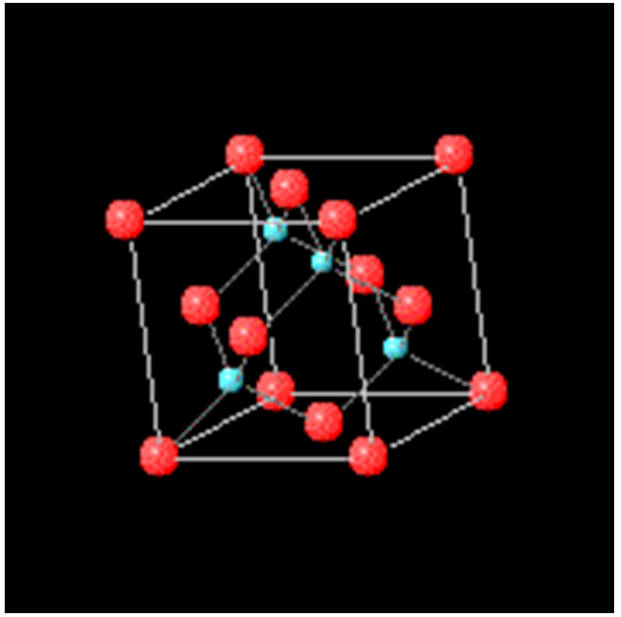
Wigner-Seitz cell ⟺ Brillouin zone

Lattice Real Space	Lattice k-space
bcc 	 fcc BZ
	bcc BZ 

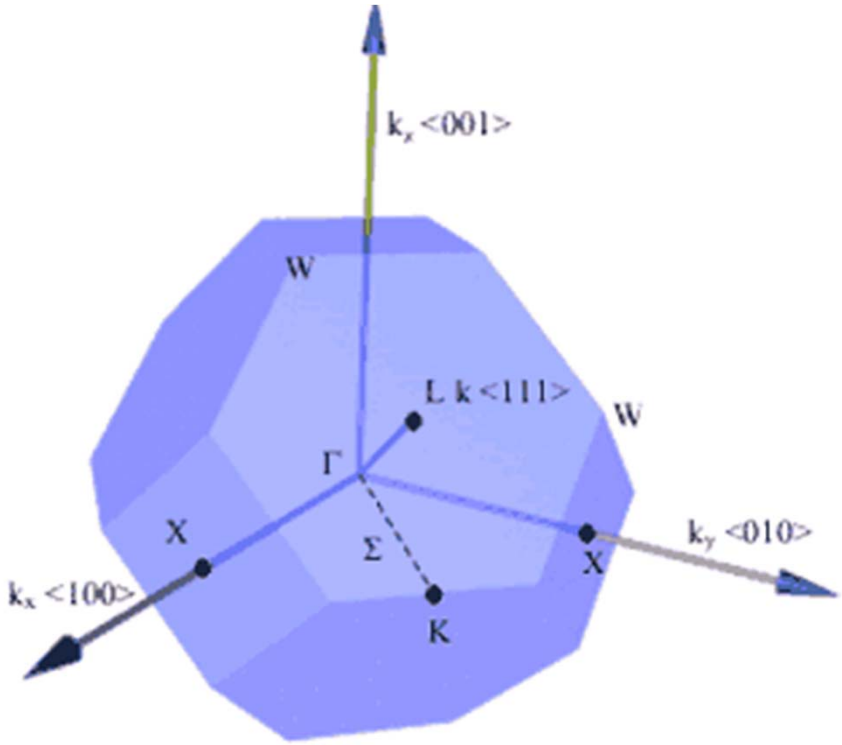
Zinc blende structure

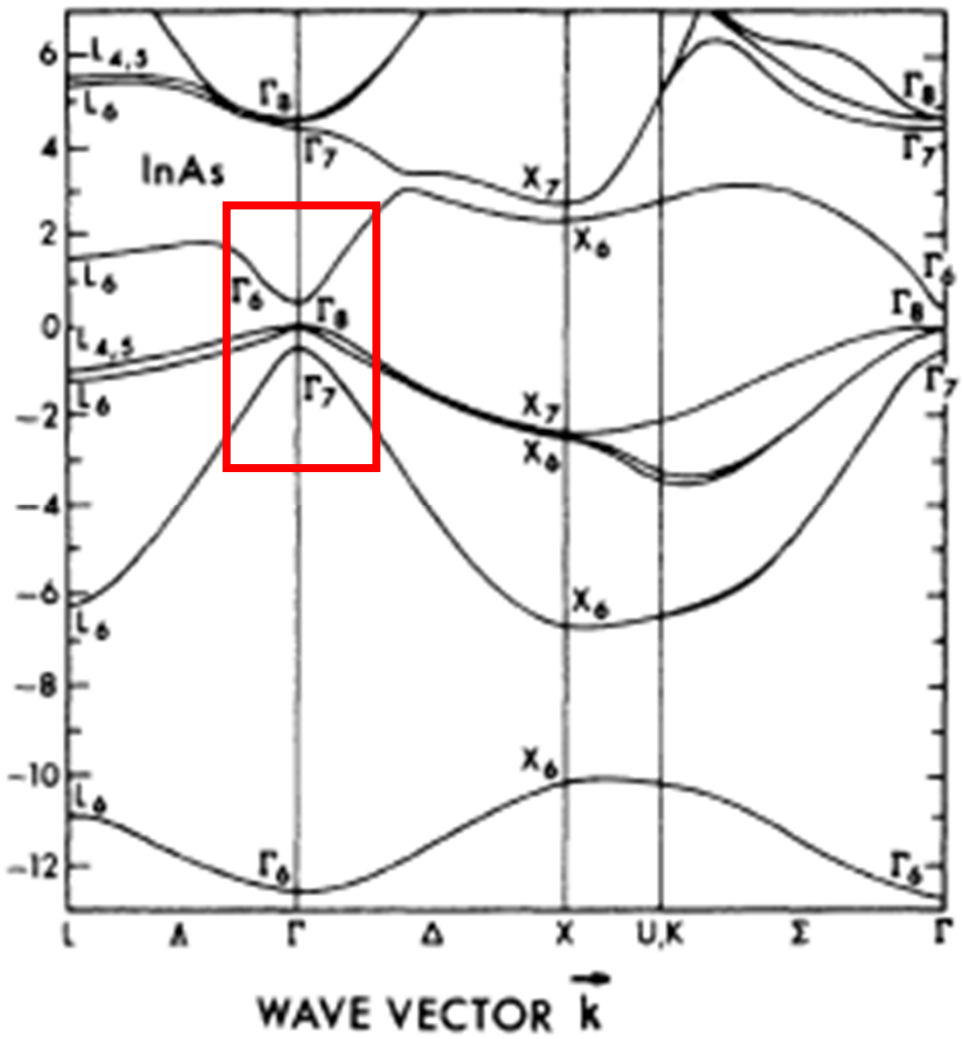
III-V semiconductors





First Brillouin Zone





We often need to know electron states only near the band extrema, where electron dispersion is close to parabolic:

m_{eff} is of arbitrary value, sign, anisotropy

$$E \approx \frac{\hbar^2 k^2}{2m_{eff}}$$

k•p method

Schroedinger's equation for a single electron in a periodic potential *V*(r):

$$\left\{\frac{p^2}{2m_0}+V(\mathbf{r})+\frac{\hbar}{4m_0^2c^2}[\nabla V\times\mathbf{p}]\cdot\sigma\right\}\psi = E\psi, \qquad \textbf{(1)}$$

$\psi = e^{i\mathbf{kr}}u_{n\mathbf{k}}(\mathbf{r})$ **- Bloch functions**

$$\hat{p}=-i\hbar\nabla \qquad p^2[u_{n\mathbf{k}}(r)\mathrm{e}^{i\mathbf{kr}}]=[(p+\hbar\mathbf{k})^2u_{n\mathbf{k}}(r)]\mathrm{e}^{i\mathbf{kr}}$$

$$\left\{\frac{p^2}{2m_0}+V(\mathbf{r})+\frac{\hbar}{4m_0^2c^2}(\sigma\times\nabla V)\cdot\mathbf{p}+\frac{\hbar^2k^2}{2m_0}+\frac{\hbar\mathbf{k}}{m_0}\cdot\left(\mathbf{p}+\frac{\hbar}{4m_0c^2}\sigma\times\nabla V\right)\right\}u_{n\mathbf{k}} =$$

$$E_{n\mathbf{k}}u_{n\mathbf{k}}. \qquad \textbf{(2)}$$

Express $u_{n\mathbf{k}}(\mathbf{r})$ **in terms of Bloch functions at k = 0:** $u_{n\mathbf{k}} = \sum_m c_m(\mathbf{k})u_{m0}.$

where $$\left[\frac{p^2}{2m_0}+V(r)\right]u_{n0}(r)=E_{n0}(r)u_{n0}(r)$$

Obtain after multiplying by $u^*_{n0}(r)$ and integrating (1) over unit cell:

$$\sum_m \left\{\left(E_{n0}-E_{m\mathbf{k}}+\frac{\hbar^2k^2}{2m_0}\right)\delta_{nm}+\frac{\hbar\mathbf{k}}{m_0}\cdot\mathbf{p}_{nm} + \frac{\hbar}{4m_0c^2}\left([\nabla V\times\mathbf{p}]\cdot\sigma+[\nabla V\times\mathbf{k}]\cdot\sigma\right)_{nm}\right\}c_m(\mathbf{k}) \;=\; 0$$

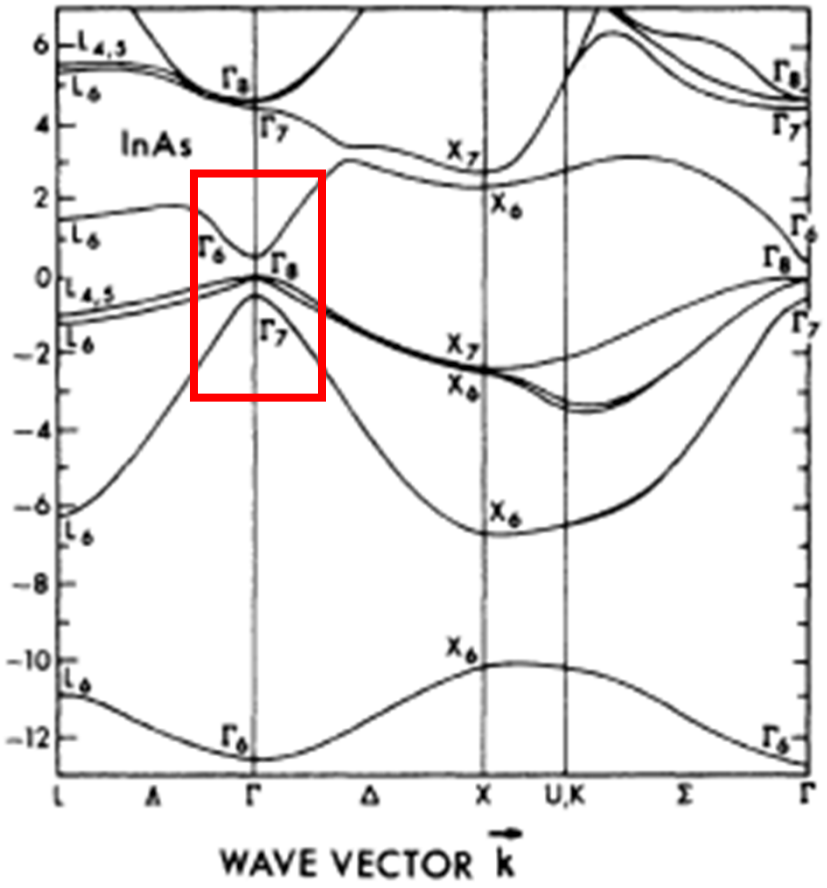
$$\mathbf{p}_{nm}=\int_{unit\,cell} u^*_{n0}(\mathbf{r})\mathbf{p}u_{m0}(\mathbf{r})d\mathbf{r}$$

Note the coupling between bands via k•p term and spin-orbit interaction

This is a matrix diagonalization problem; however it is still too complicated because of too many bands

Next step: Lowdin's perturbation method to reduce the size of the problem

Only closest bands are included (e.g. 8 bands)

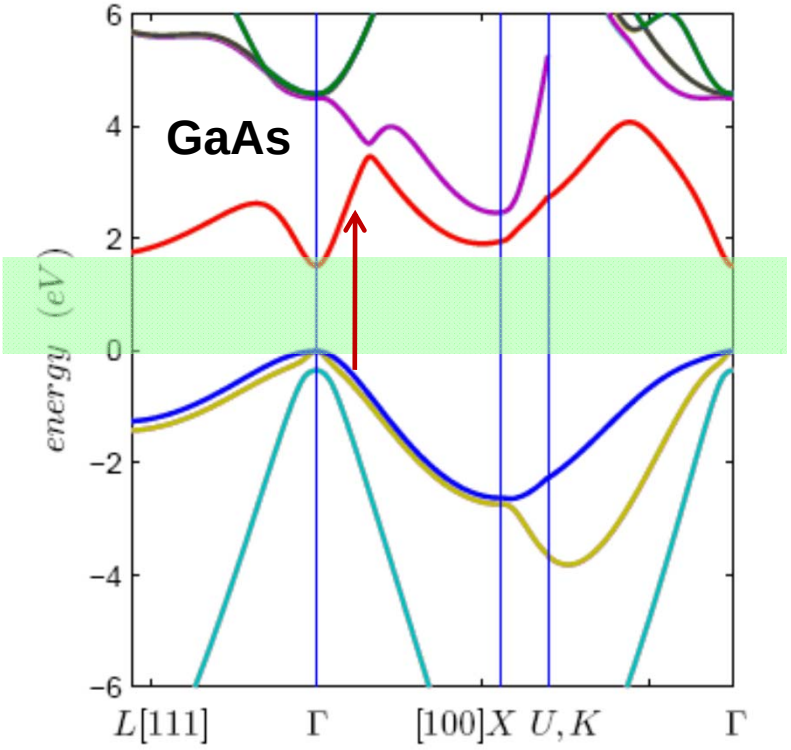


The Luttinger-Kohn basis for u_{n0}(r) states:

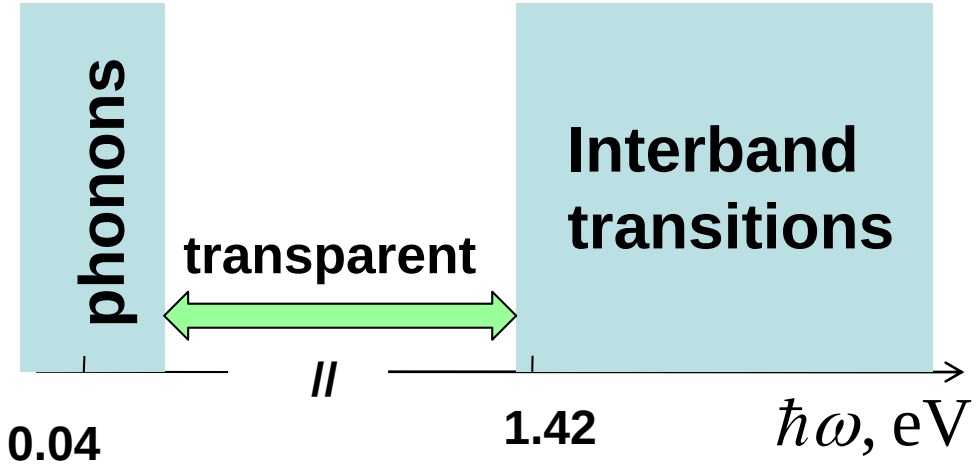
	$\lvert J, m_J\rangle$	ψ	$H(k=0)$
CB		$S\uparrow$	E_g
		$S\downarrow$	E_g
HH	$\lvert 3/2, 3/2\rangle$	$\left(\frac{X+iY}{\sqrt{2}}\right)\uparrow$	0
	$\lvert 3/2, -3/2\rangle$	$-\frac{1}{\sqrt{2}}(X-iY)\downarrow$	0
LH	$\lvert 3/2, 1/2\rangle$	$-\sqrt{\frac{2}{3}}Z\uparrow+\frac{1}{\sqrt{6}}(X+iY)\downarrow$	0
	$\lvert 3/2, -1/2\rangle$	$-\frac{1}{\sqrt{6}}(X-iY)\uparrow-\sqrt{\frac{2}{3}}Z\downarrow$	0
SO	$\lvert 1/2, 1/2\rangle$	$\frac{1}{\sqrt{3}}(X+iY)\downarrow+\frac{1}{\sqrt{3}}Z\uparrow$	$-\Delta$
	$\lvert 1/2, -1/2\rangle$	$-\frac{1}{\sqrt{3}}Z\downarrow+\frac{1}{\sqrt{3}}(X-iY)\uparrow$	$-\Delta$

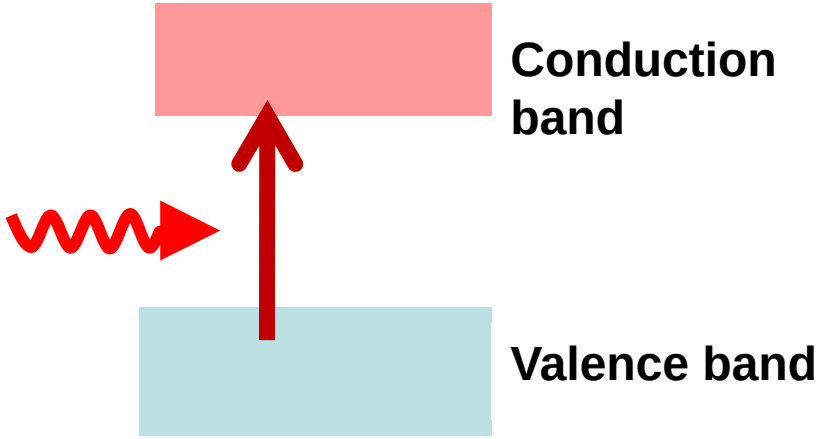
S,X,Y,Z **are similar to S-like and P-like atomic states (lowest order spherical harmonics Y_{00}, Y_{10}, Y_{11} etc.)**

Bulk intrinsic semiconductors can only absorb light

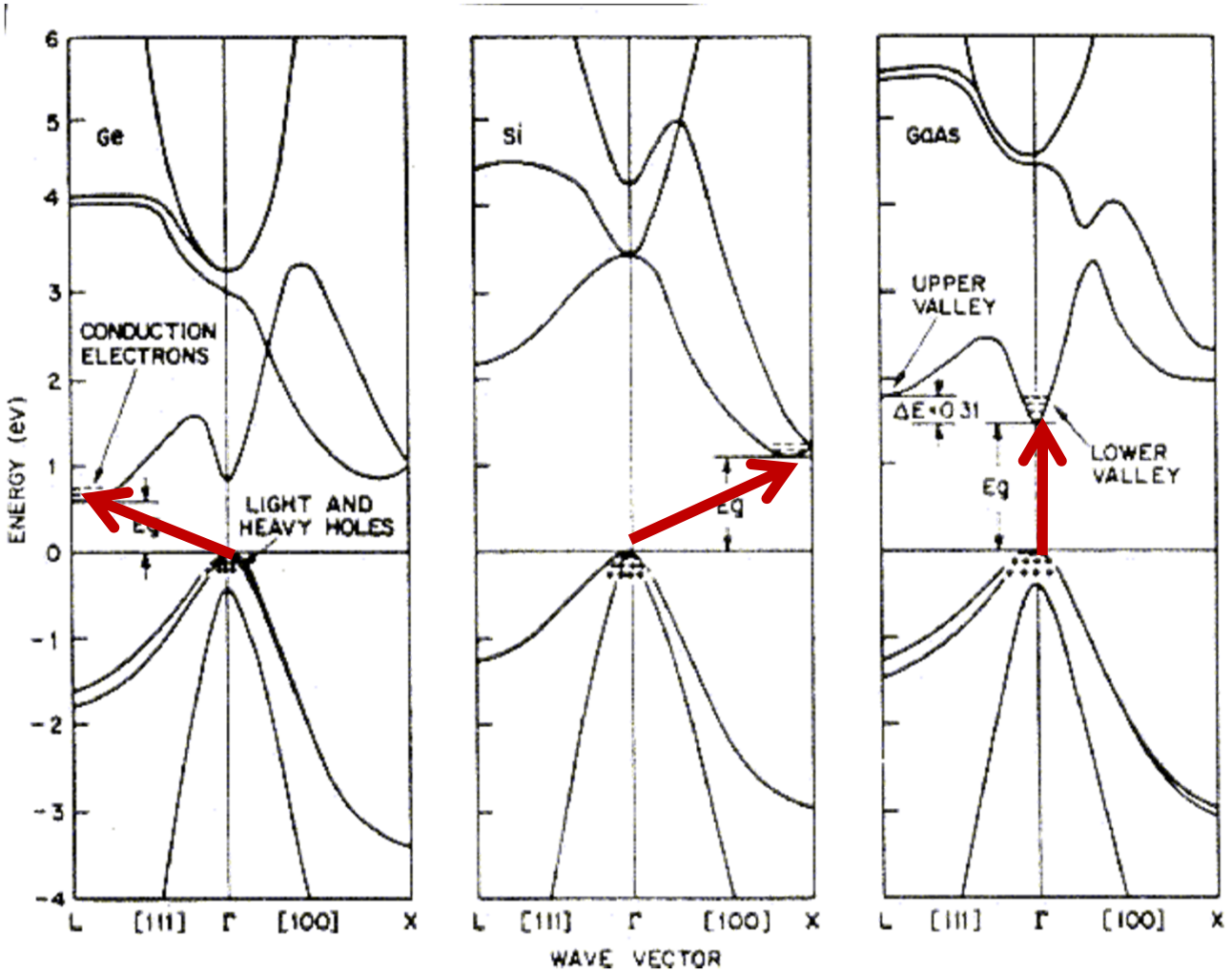


30-band kP method



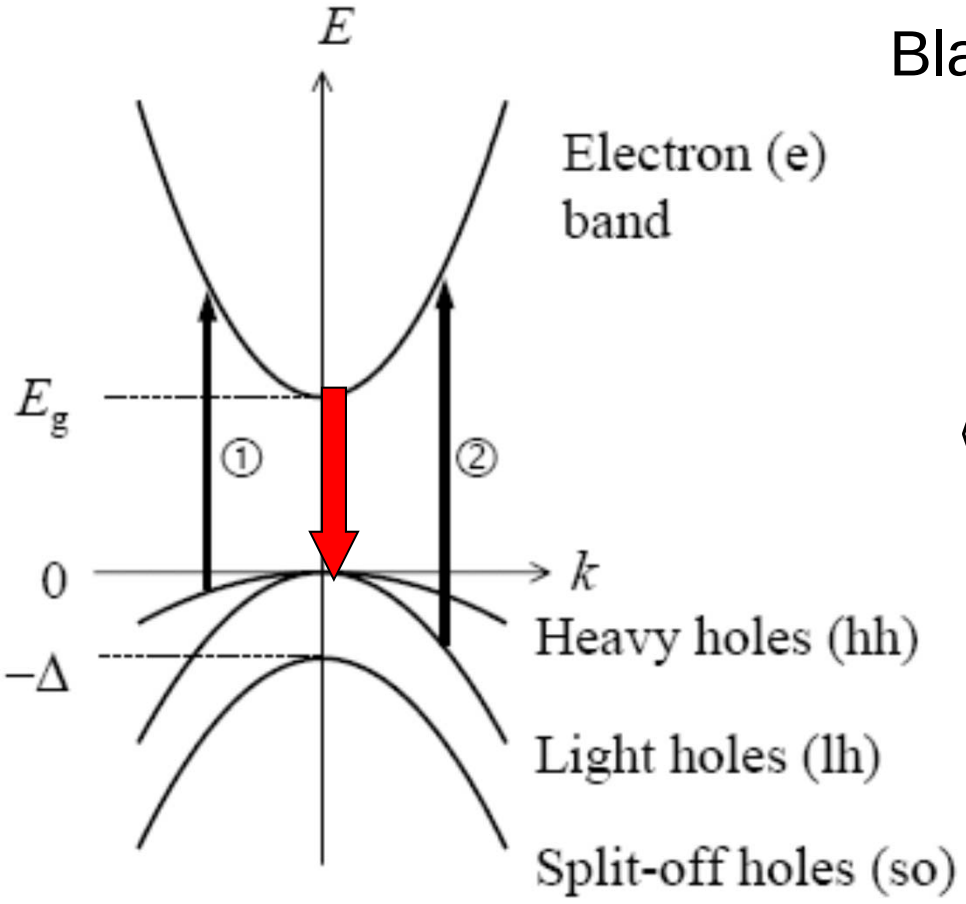


Indirect-gap versus direct-gap semiconductors



germanium silicon GaAs

Interband transitions



Blackboard derivation

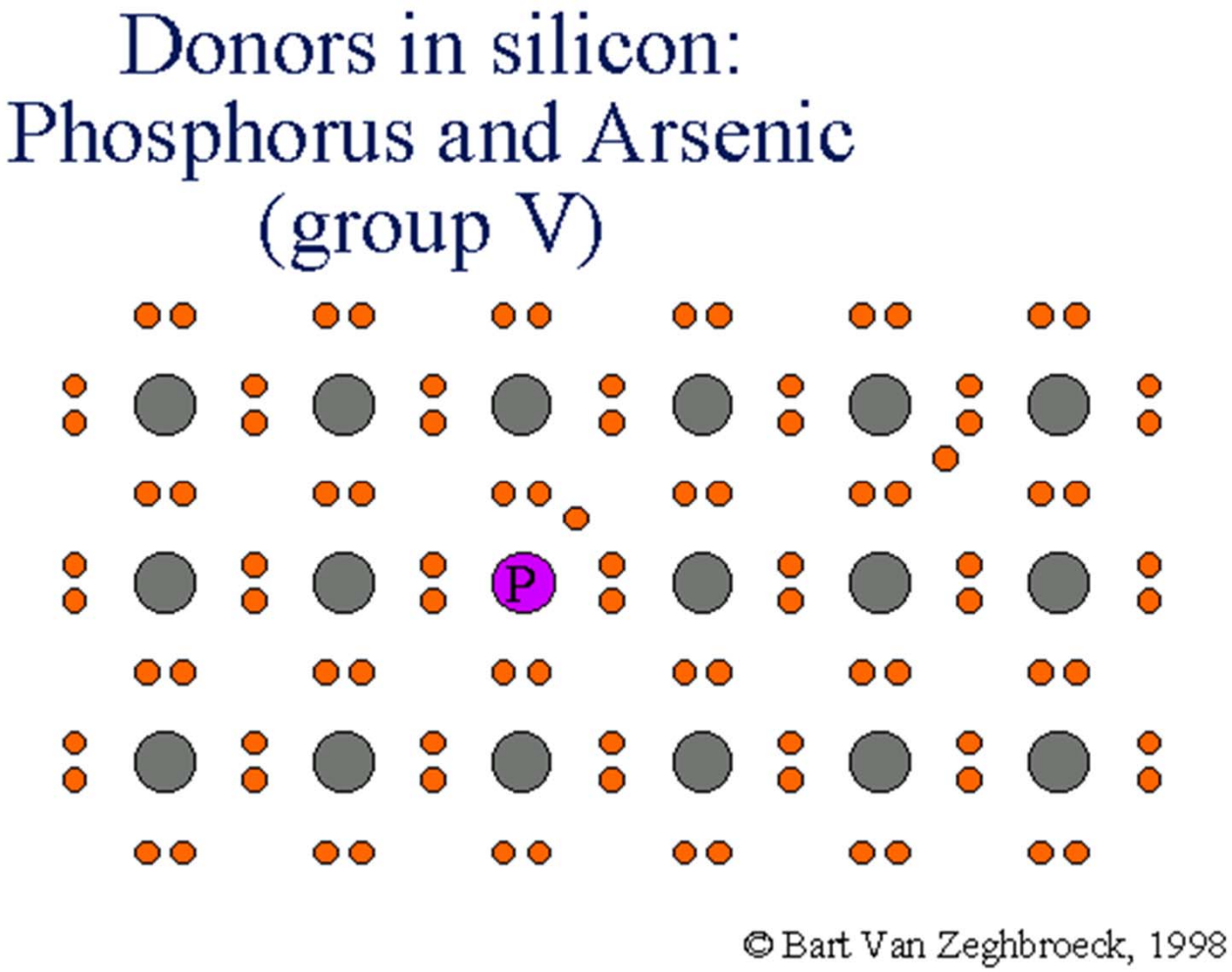
$$\hat{V}_{EM} = -(q/c)A\hat{p}$$

$$\left\langle \psi_{n',k'} \middle| V \middle| \psi_{n,k} \right\rangle \propto p_{n'n}\delta_{k'k}$$

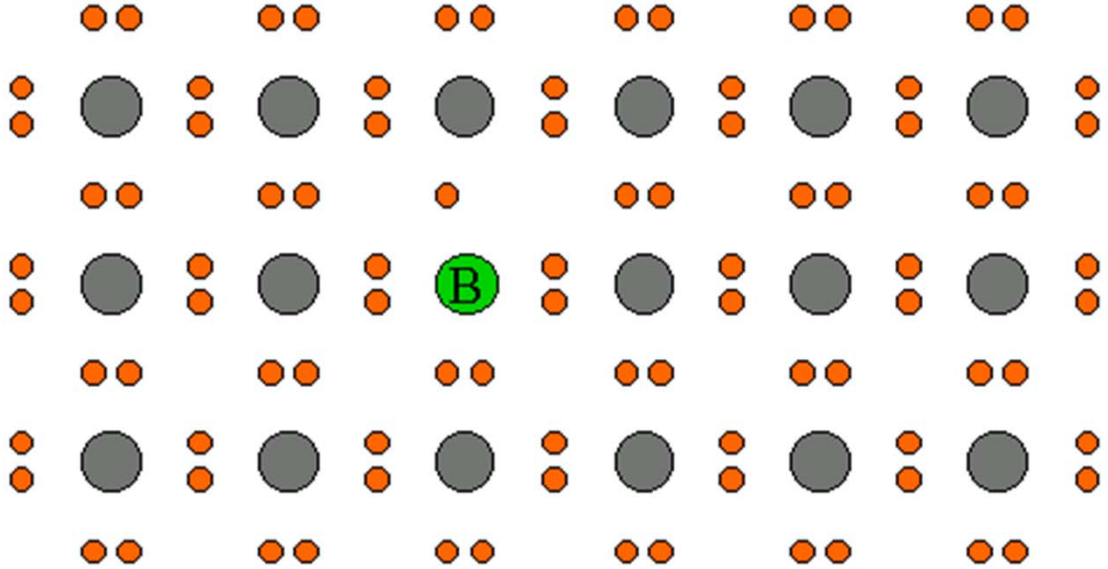
Need to calculate matrix element $p_{n'n}$ and know density of states and their occupation

Density of states: blackboard derivation

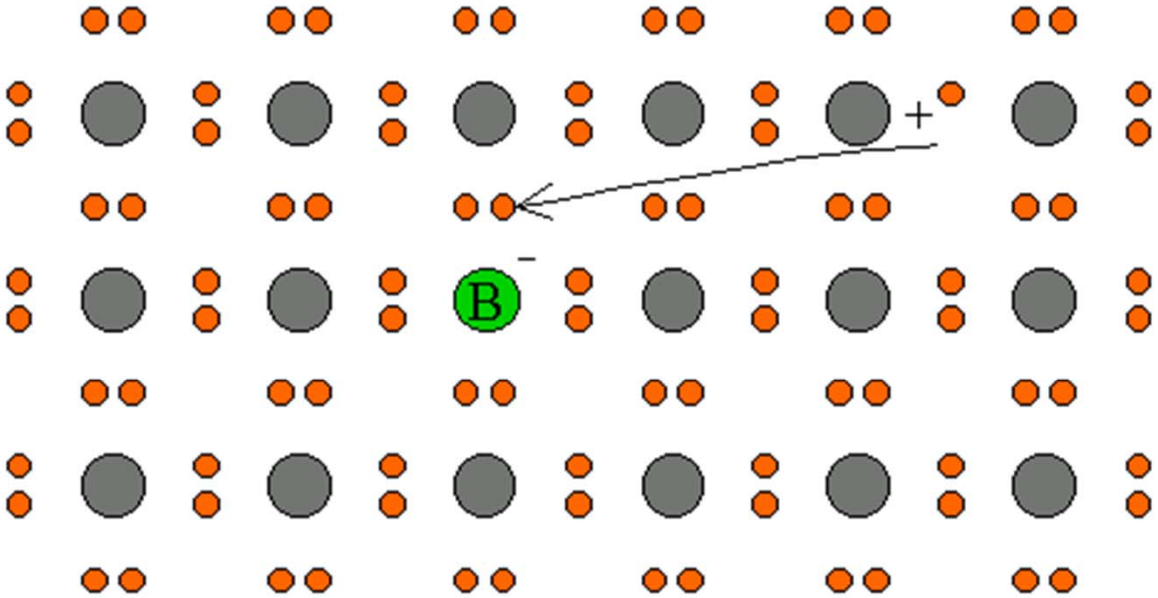
The best thing about semiconductors: they can be doped



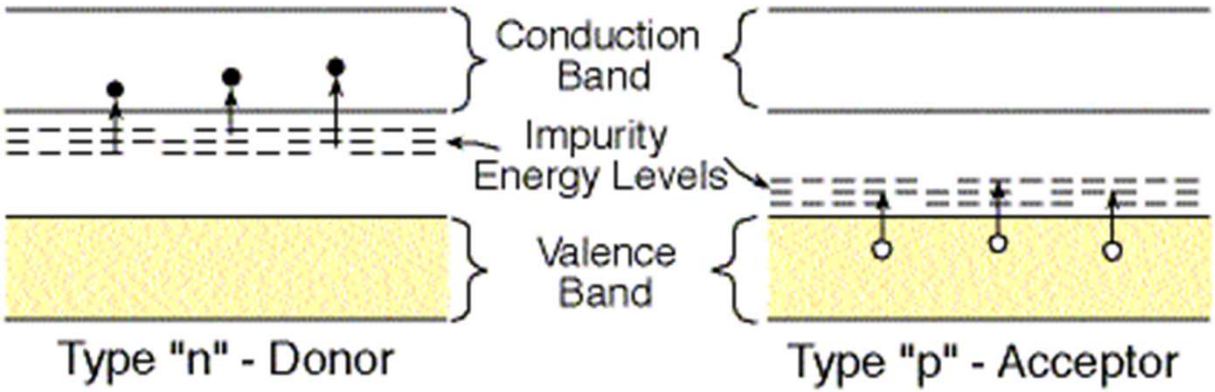
Acceptors in silicon: Boron (group III)



Ionization of acceptors

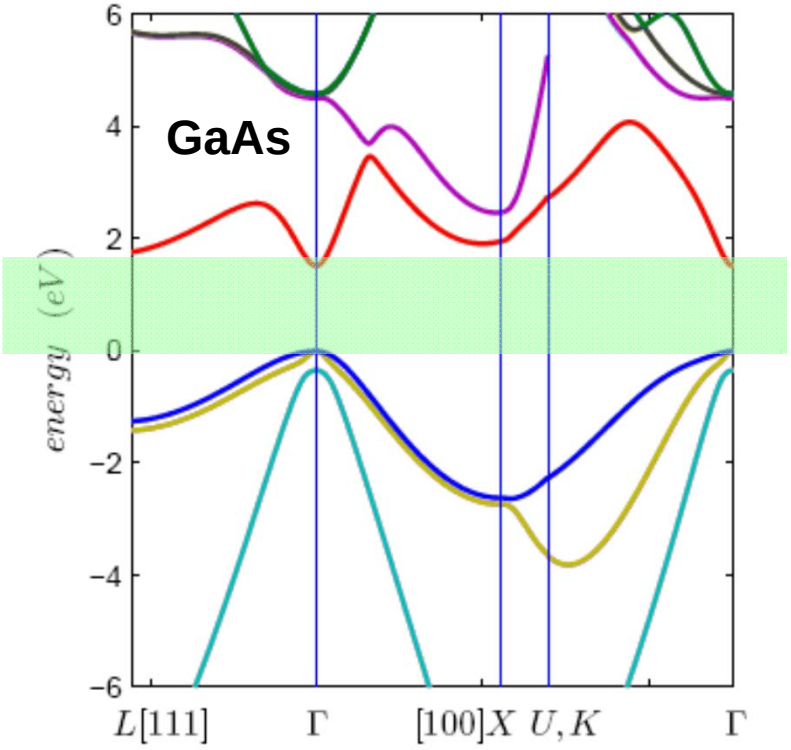


Small amount of impurities (dirt) leads to huge changes in conductivity;
Both negative and positive current carriers are possible

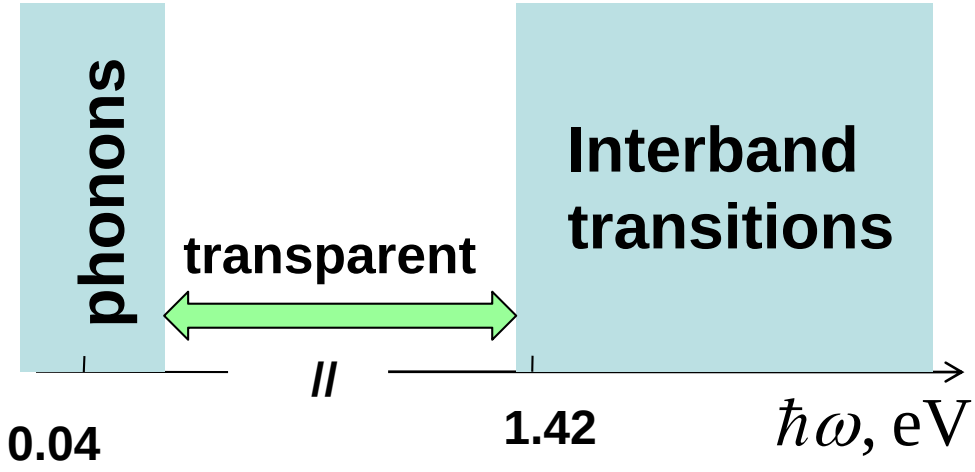


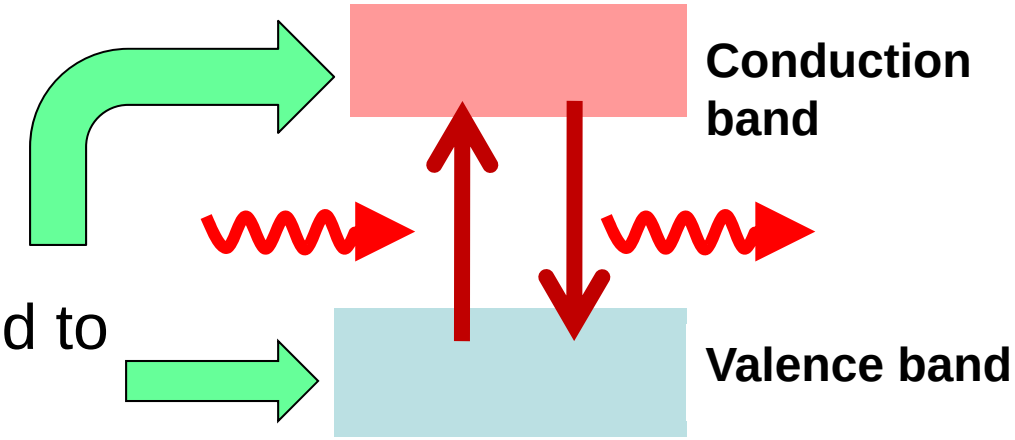
Revolution in the way we process information:
Enabled by transistors, memory, computers, lasers, telecommunications

Doping enabled optoelectronic devices

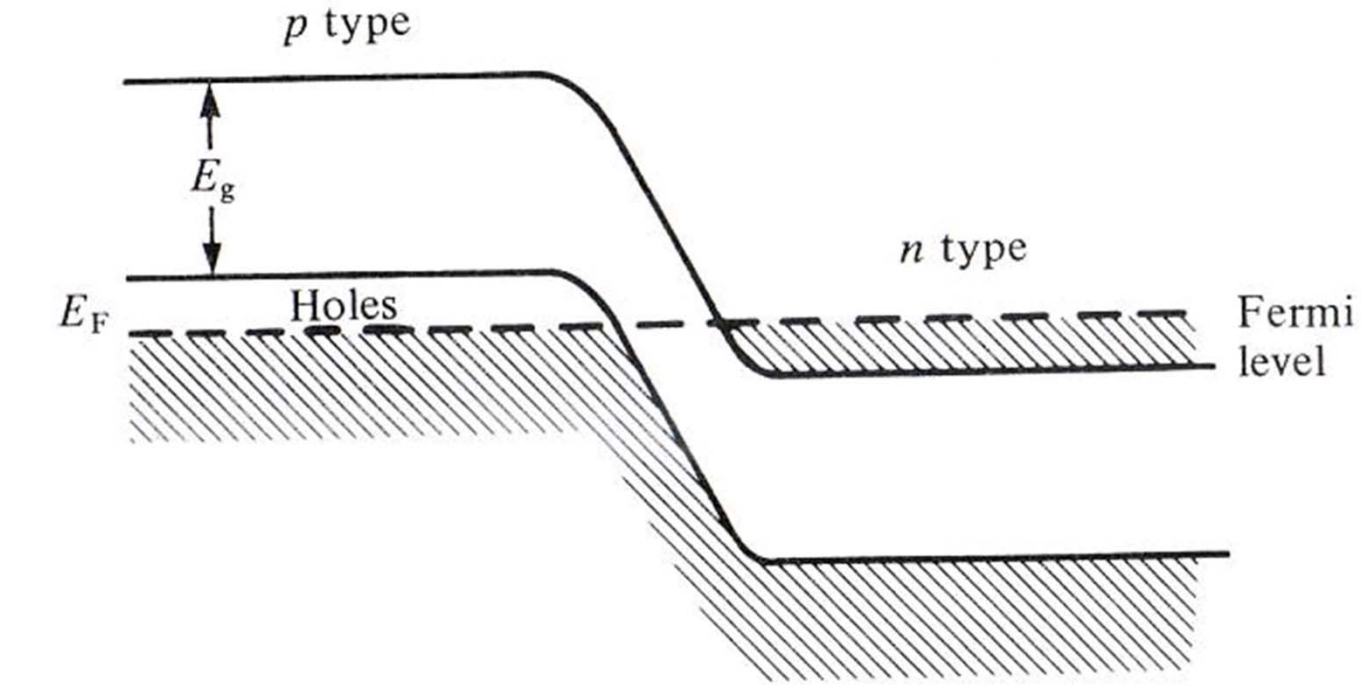


Y.Cho, 30-band kP method





To generate light, you need to inject electrons and holes



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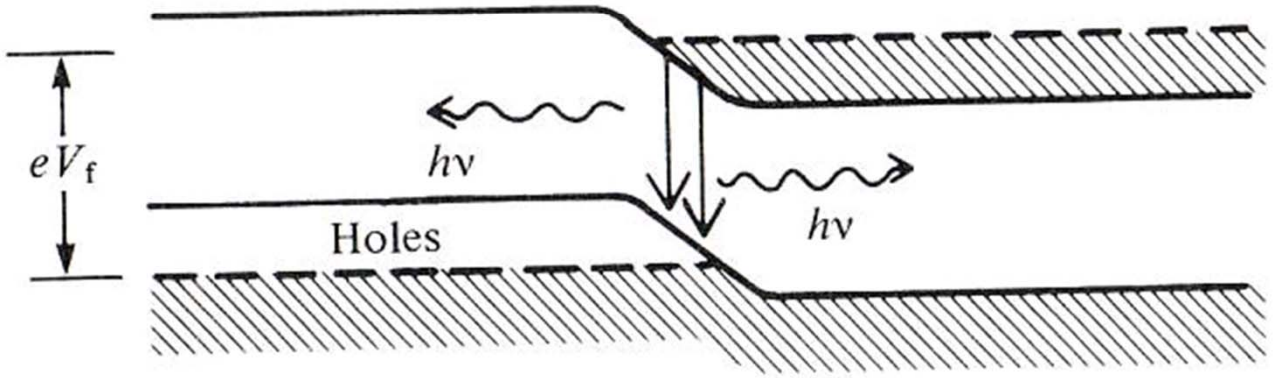

(b)