Band Theory, local and non-local states

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International School and Conference on Functional Materials for Modern Technologies
October 1-7, Batumi Georgia

Why Band Theory?

All properties of solid-state materials and all their functionality are conditioned by bandstructure – electronic structure - energies and wavefunctions of electrons

Outline of the lecture

- **Quantum state and Schrodinger equation**
- **Crystal symmetry**
- **Free electron model**
- **Nearly free electron model**
- **Tight binding k•p theory, effective mass**

Quantum vs classical description

Classical Description

- $\vec{r}(t), \vec{v}(t)$
- $m\frac{d^2\vec{r}}{dt^2} = \vec{F}$
- All quantities can be measured

Quantum Description

- $\Psi(\vec{r}, t)$
- Only the **quantities which are conserved** can be measured doubtlessly, their values are defined by **quantum numbers**

Discrete of continues

$\boldsymbol{\Psi(\vec{r}, t)dV}$ **– probability of finding particle in a small volume dV around the r**

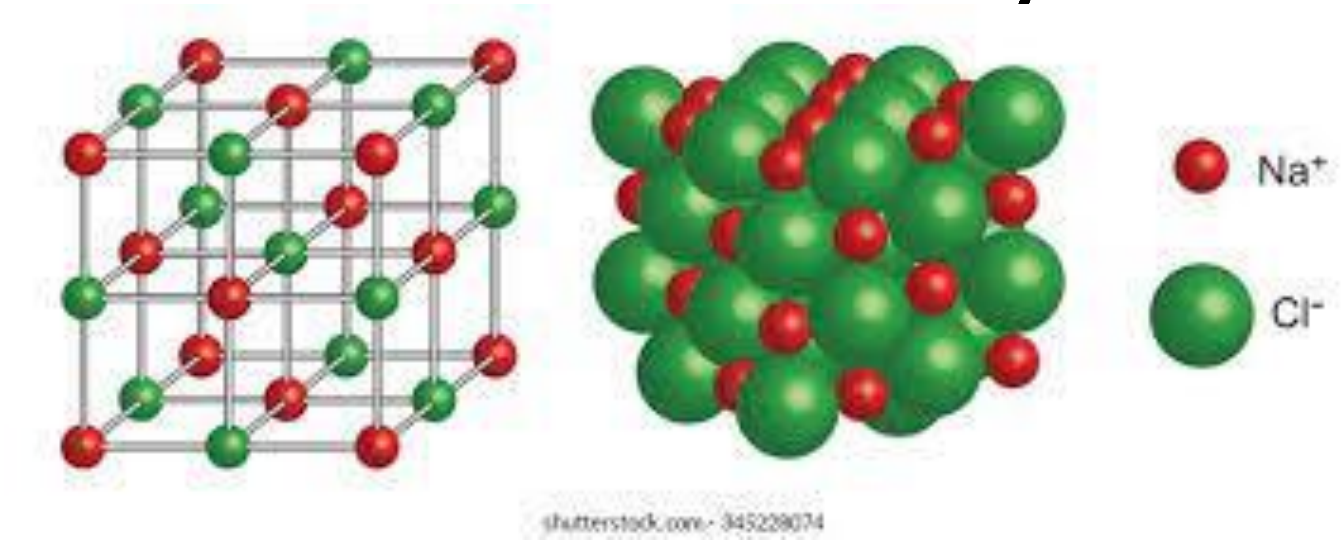
The Schrodinger equation

Potential energy

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi$$

Both to be found

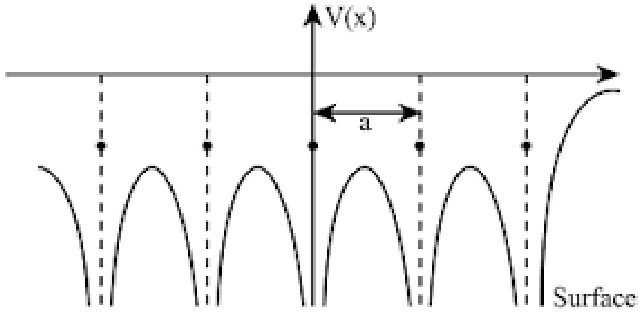
Crystals



The electron states in the presence of many (ordered) atoms(ions) to be found

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi$$

To be solved for periodic potential



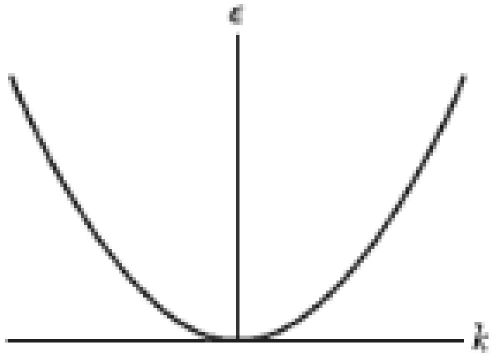
Simplest model – particle in a box

$$\Psi_k\left(\vec{r}\right) = e^{i\vec{k}\vec{r}} .$$

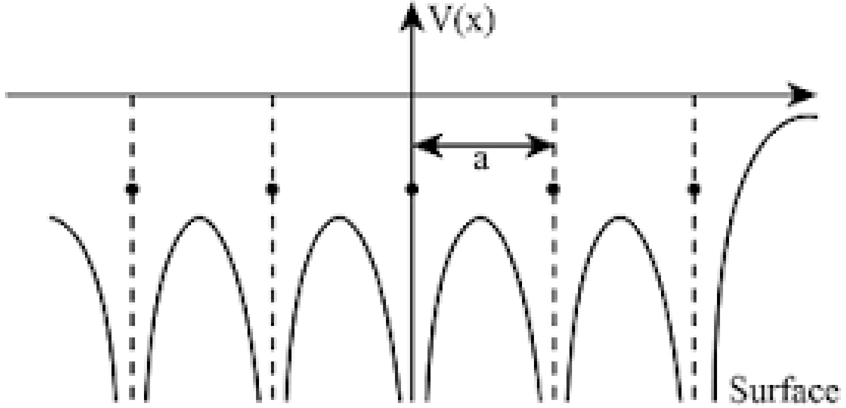
$$E_k = \frac{\hbar^2}{2m}\left(k_x^{\,2} + k_y^{\,2} + k_z^{\,2}\right)$$

$$\psi\left(x+L, y, z\right) = \psi\left(x, y+L, z\right) = \psi\left(x, y, z+L\right) = \psi\left(x, y, z\right)$$

$$k_x, k_y, k_z = 0; \pm\frac{2\pi}{L}; \pm\frac{4\pi}{L} .....$$

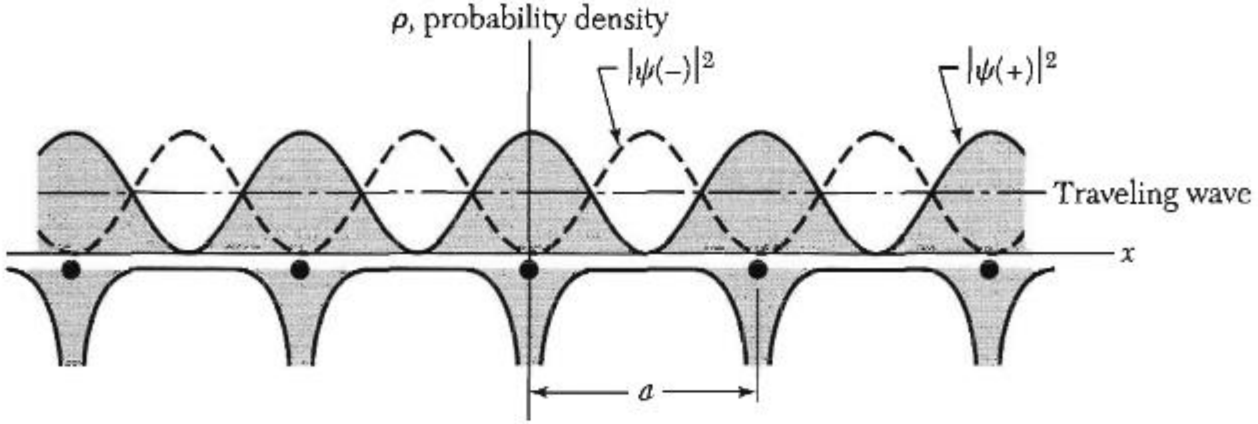


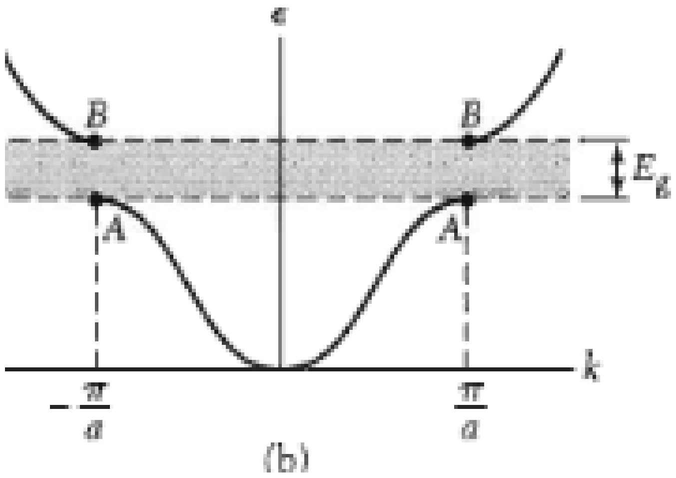
Nearly free electron model



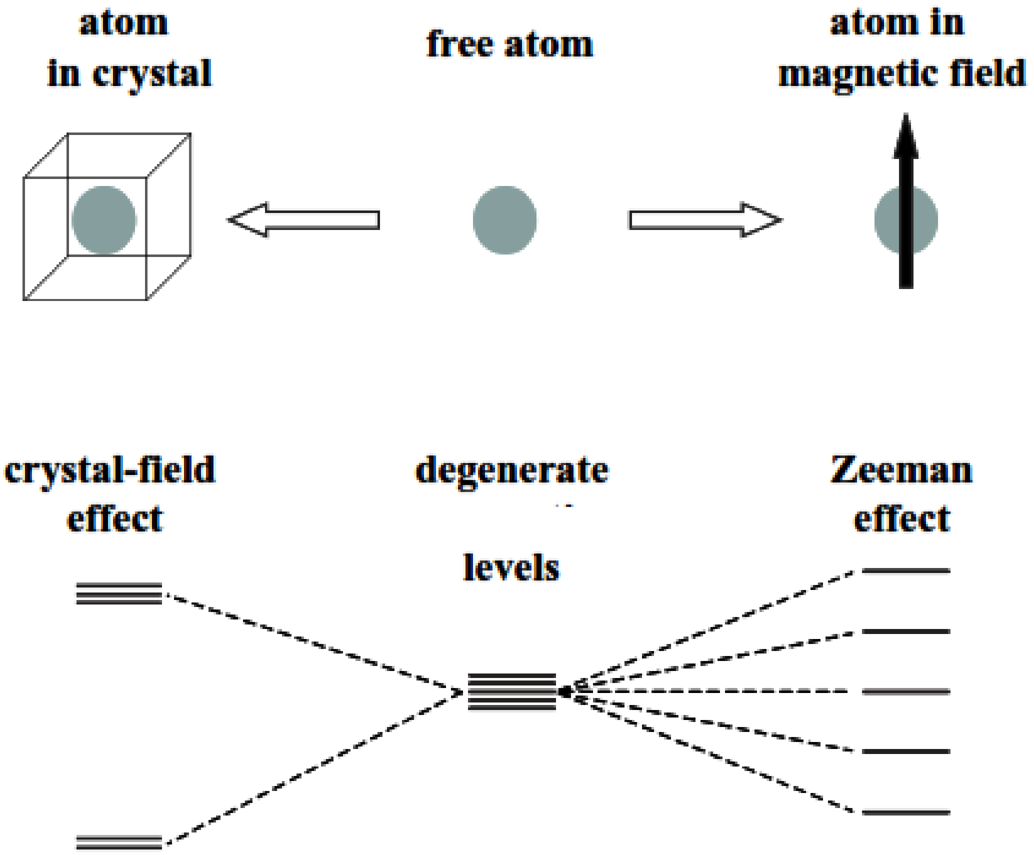
$$\psi(+) = e^{i\pi x/a} + e^{-i\pi x/a} = 2\cos\frac{\pi x}{a} \qquad \rho(+) = |\psi(+)|^2 \sim \cos^2\frac{\pi x}{a}$$

$$\psi(-) = e^{i\pi x/a} - e^{-i\pi x/a} = 2i\sin\frac{\pi x}{a} \qquad \rho(-) = |\psi(-)|^2 \sim \sin^2\frac{\pi x}{a}$$





Crystal symmetry



Band Structure of Semiconductors

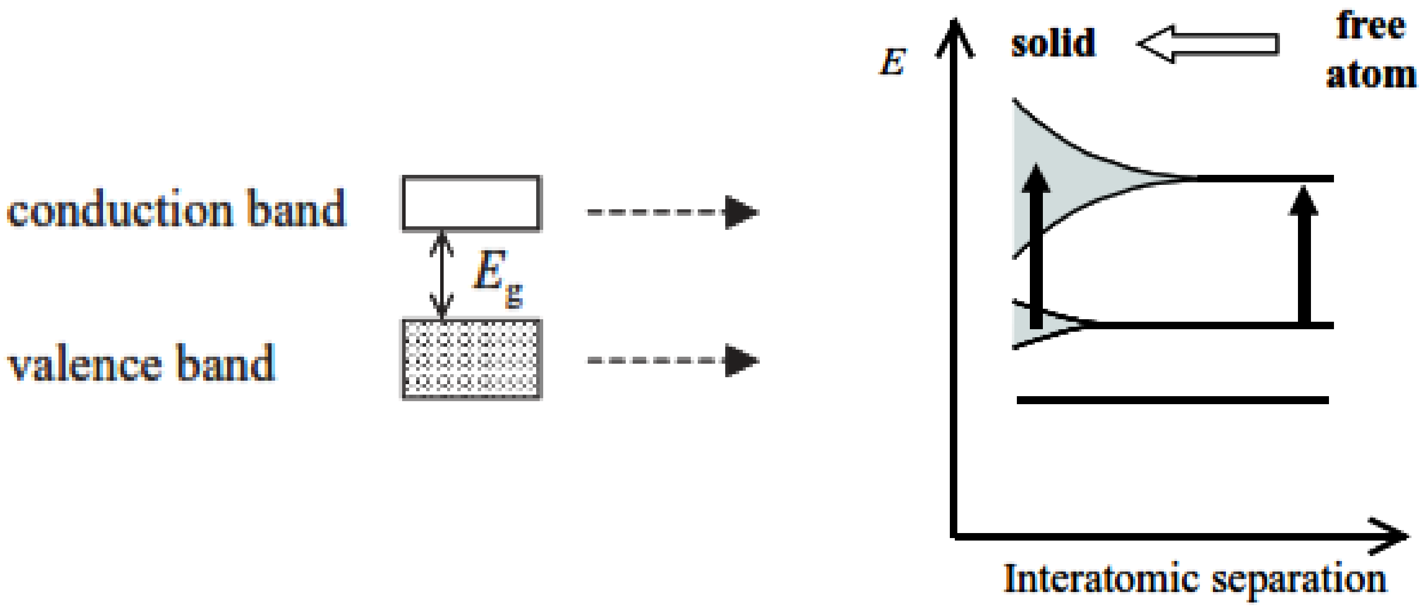
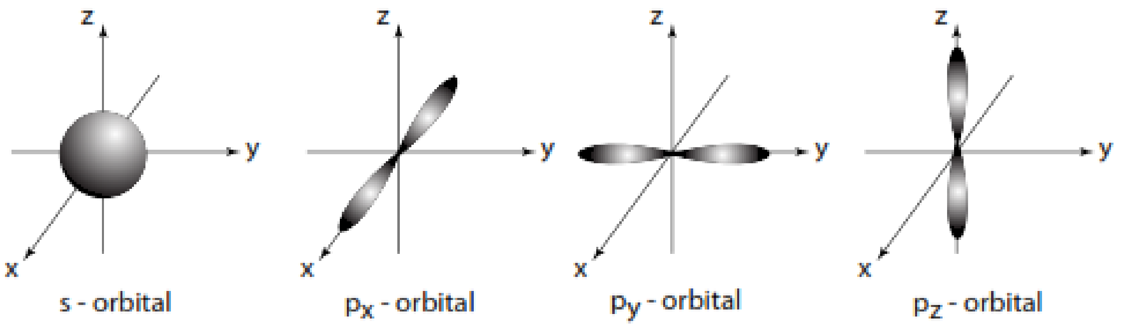


Fig. 3 Formation of energy bands

- **New quantum number quasi momentum appears (quasi wave vector) – as quantum states inside the band have different quasi momentum**
- **Interaction with lattice vibrations (Phonons)**

kp method

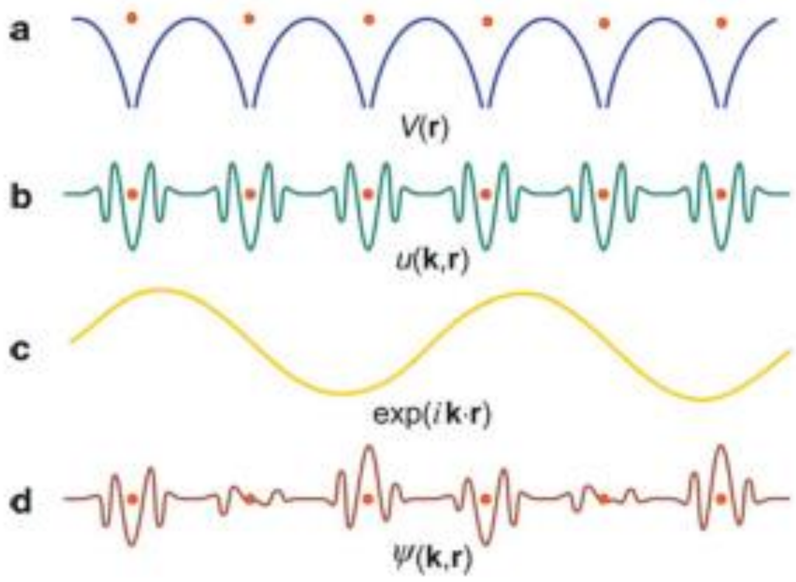
- 1. Find the dispersion E-k dependence for small k
- 2. Find electron wave function in crystal using atomic wave functions



Periodic potential

$$\left[-\frac{\hbar^2}{2m}\Delta + V(\vec{r})\right]\Psi(\vec{r}) = E(\vec{k})\Psi(\vec{r})$$

$$\Psi_{nk}(\vec{r}) = e^{i\vec{k}\vec{r}}u_{nk}(\vec{r})$$



Bloch function

$$u_{nk}(\vec{r}) = u_{nk}(\vec{R}+\vec{n})$$

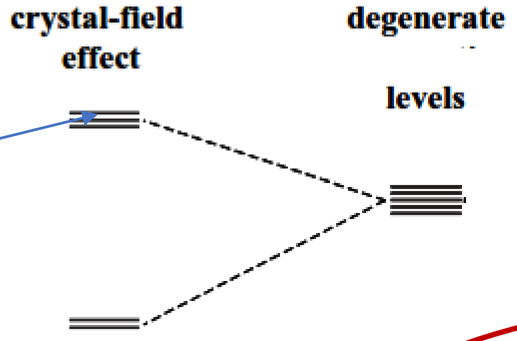
$$\left[-\frac{\hbar^2}{2m}\Delta+V(\vec{r})\right]\Psi_{nk}(\vec{r})=E_n(\vec{k})\Psi_{nk}(\vec{r}) \ .$$

$$\left[-\frac{\hbar^2}{2m}\Delta+V(\vec{r})\right]e^{i\vec{k}\vec{r}}u_{nk}(\vec{r})=E_n(\vec{k})e^{i\vec{k}\vec{r}}u_{nk}(\vec{r})$$

$$\left[-\frac{\hat{p}^2}{2m}+V(\vec{r})+\frac{\hbar}{m}\left(\vec{k}\hat{p}\right)\right]u_{nk}(\vec{r})=\left(E_n(\vec{k})-\frac{\hbar^2k^2}{2m}\right)u_{nk}(\vec{r}) \ .$$

Perturbation

$$\left[\hat{H}_0+\frac{\hbar}{m}\left(\vec{k}\hat{p}\right)\right]u_{nk}(\vec{r})=\left(E_n(\vec{k})-\frac{\hbar^2k^2}{2m}\right)u_{nk}(\vec{r})$$



$$E_{nk} = E_{n0} + \frac{\hbar^2 k^2}{2m^*}$$

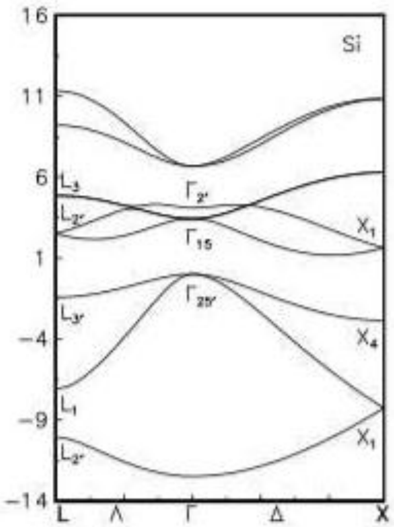
$$H_0 = -\frac{\hat{p}^2}{2m} + V(\vec{r})$$

$$\vec{k}\cdot\hat{p} = k_x\left(i\hbar\frac{\partial}{\partial x}\right) + k_y\left(i\hbar\frac{\partial}{\partial y}\right) + k_z\left(i\hbar\frac{\partial}{\partial z}\right)$$

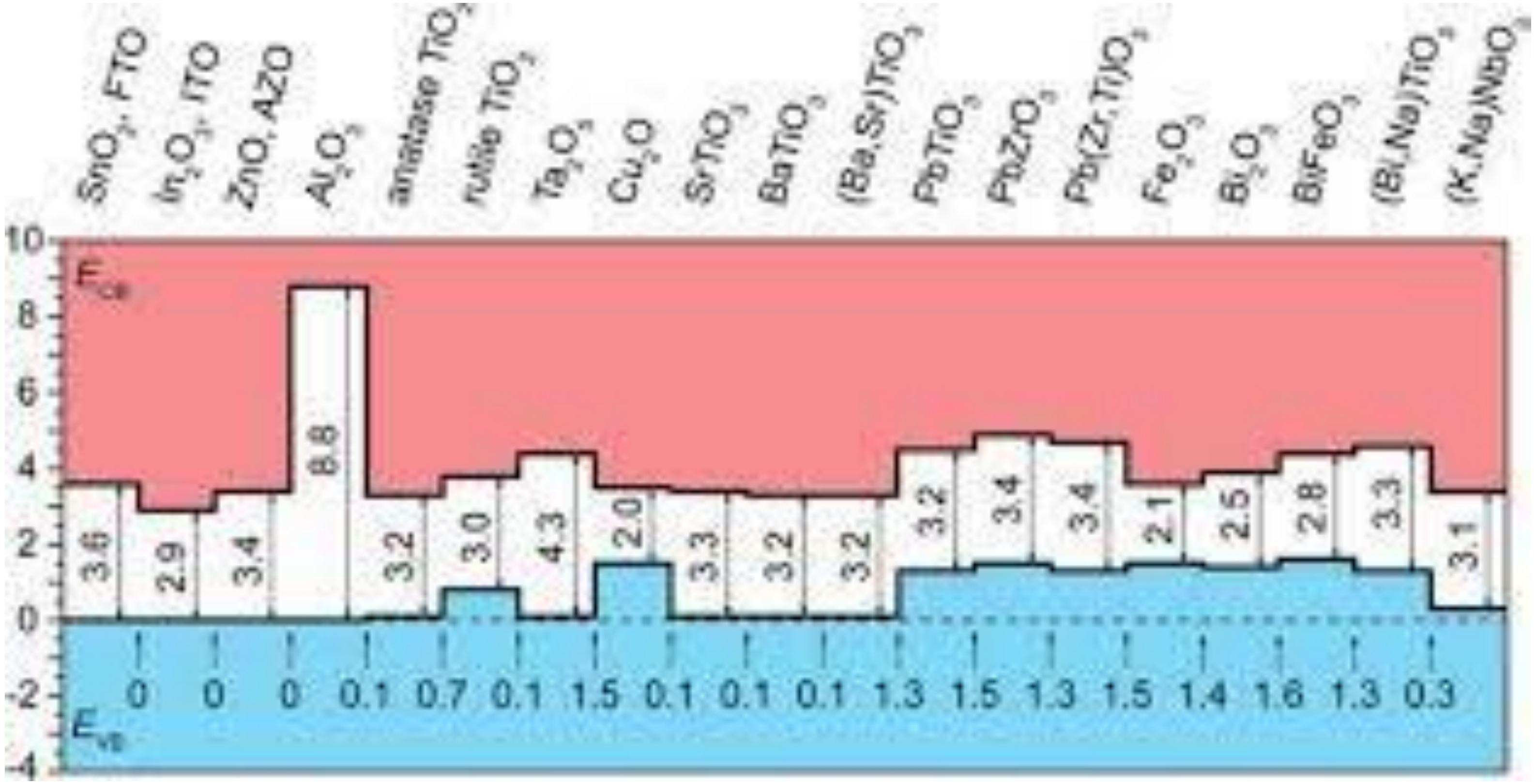
$$\frac{1}{m^*} = \frac{1}{m}\left[1 + \frac{2}{mk^2}\right]\sum_{n\neq n'}\frac{\left|\langle u_{n0}|\vec{k}p|u_{n'0}\rangle\right|^2}{E_{no} - E_{n'0}}$$

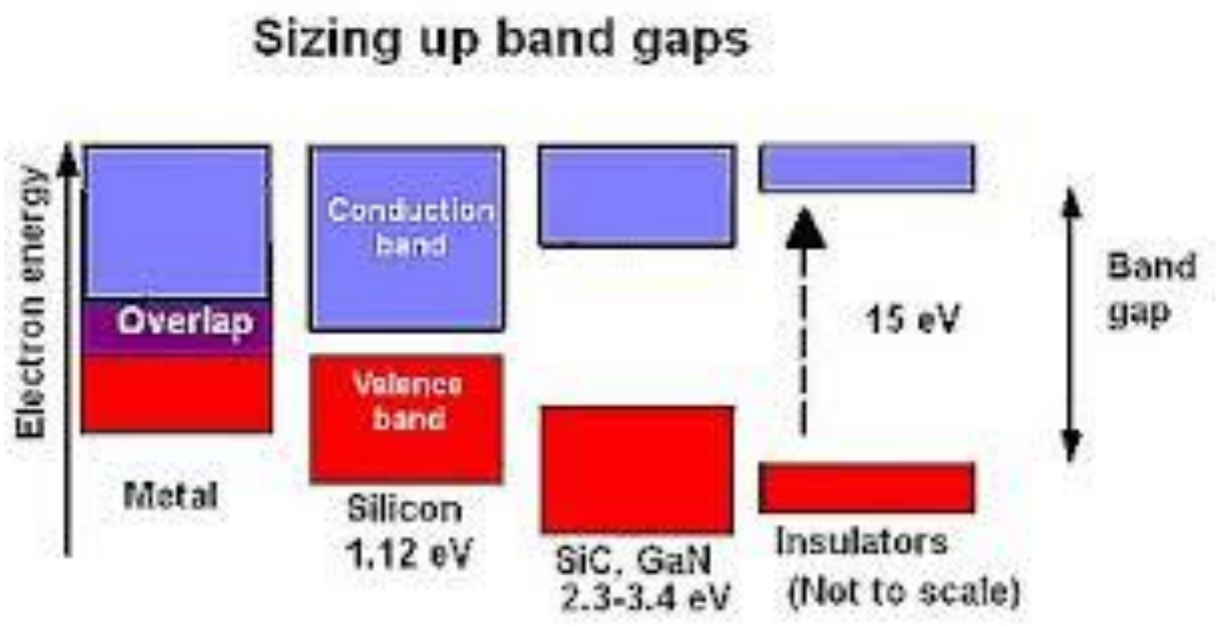
$$E_{nk} = E_{n0} + \frac{\hbar^2 k^2}{2m} + \frac{\hbar^2}{m^2}\sum_{n\neq n'}\frac{\left|\langle u_{n0}|\vec{k}p|u_{n'0}\rangle\right|^2}{E_{no} - E_{n'0}}$$

$$u_{nk} = u_{n0} + \frac{\hbar}{m}\sum_{n\neq n'}\frac{\langle u_{n0}|\vec{k}p|u_{n'0}\rangle}{E_{no} - E_{n'0}}$$



Band Alignment





Sizing up band gaps
Electron energy
Overlap
Metal
Conduction band
Valence band
Silicon
1.12 eV
SiC, GaN
2.3-3.4 eV
15 eV
Insulators
(Not to scale)
Band gap

Thank you for Attention!