Fundamentals of Solid State Physics

Electronic Band - Summary

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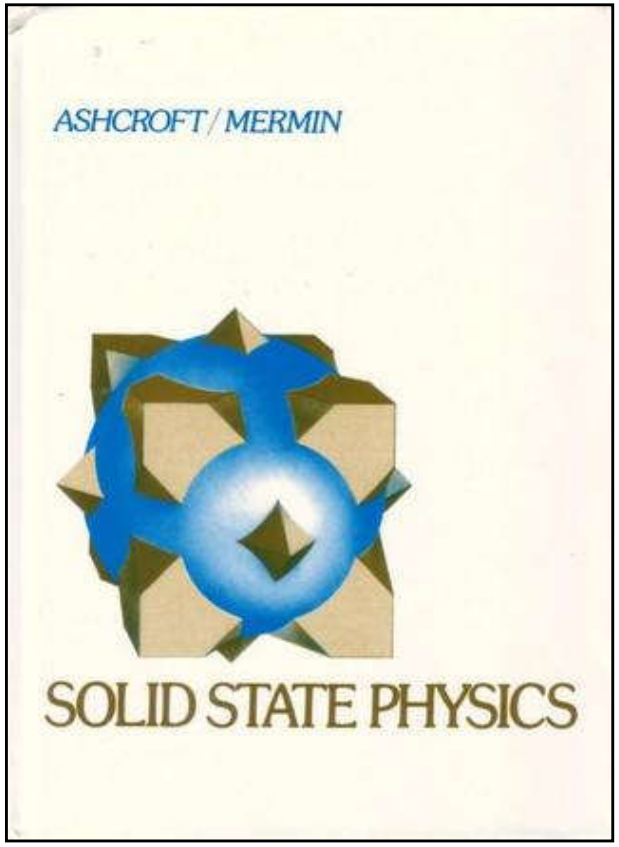
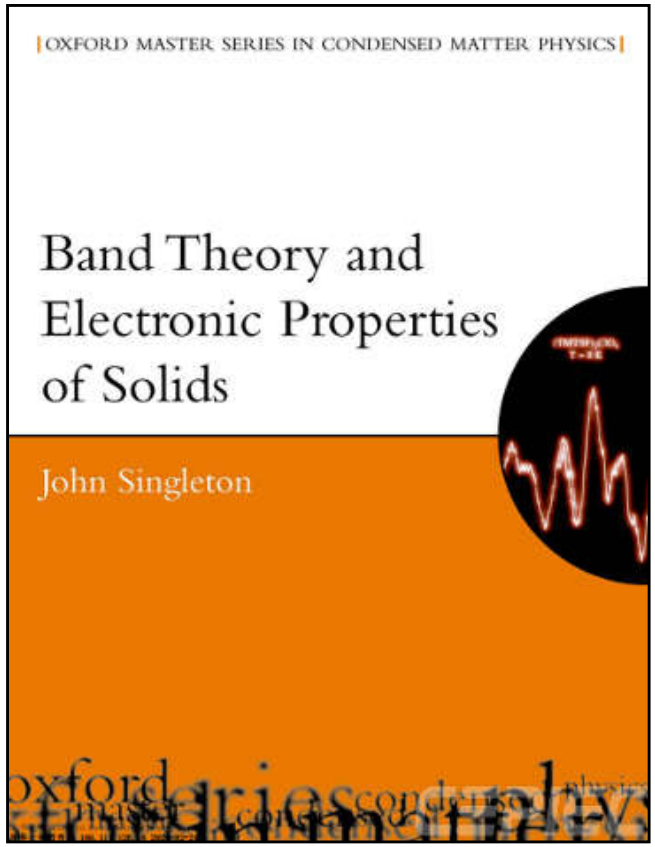
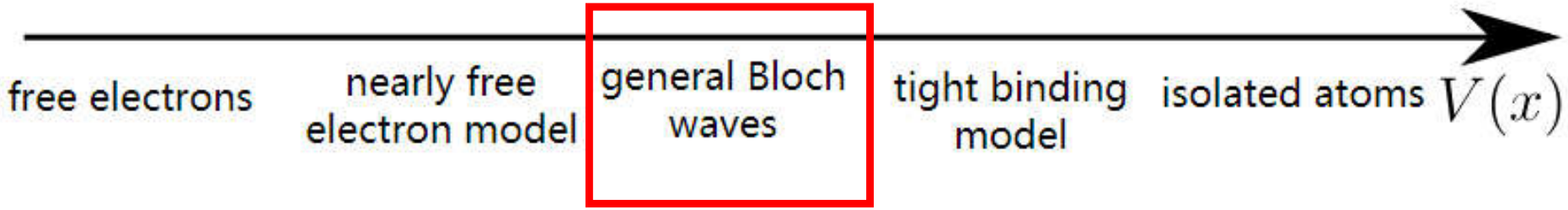
Further Reading

- **Singleton, Chapter 5**
- **Ashcroft & Mermin, Chapter 12, 13**

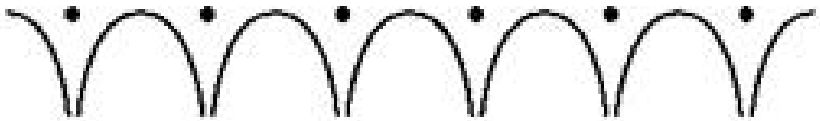




Summary



$V(\mathbf{r})$

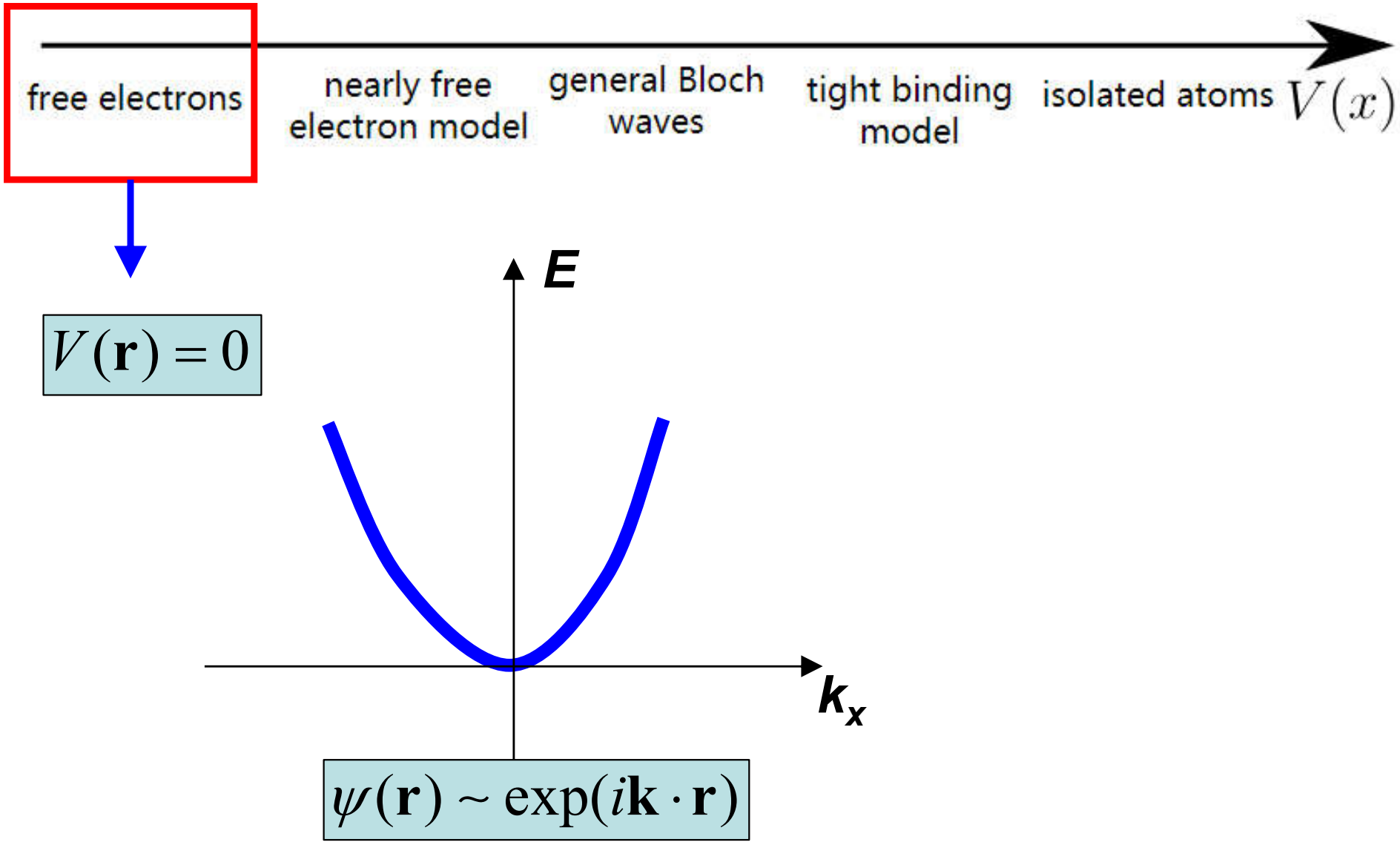


electrons in a periodic potential

$$\psi(\mathbf{r}) = \exp(i\mathbf{k}\cdot\mathbf{r})\cdot u_{\mathbf{k}}(\mathbf{r})$$

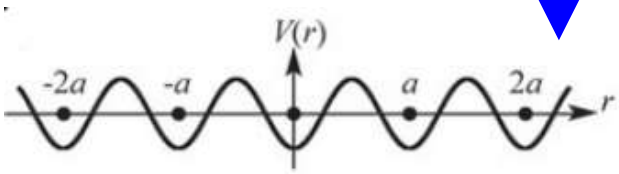
Bloch wave

Summary

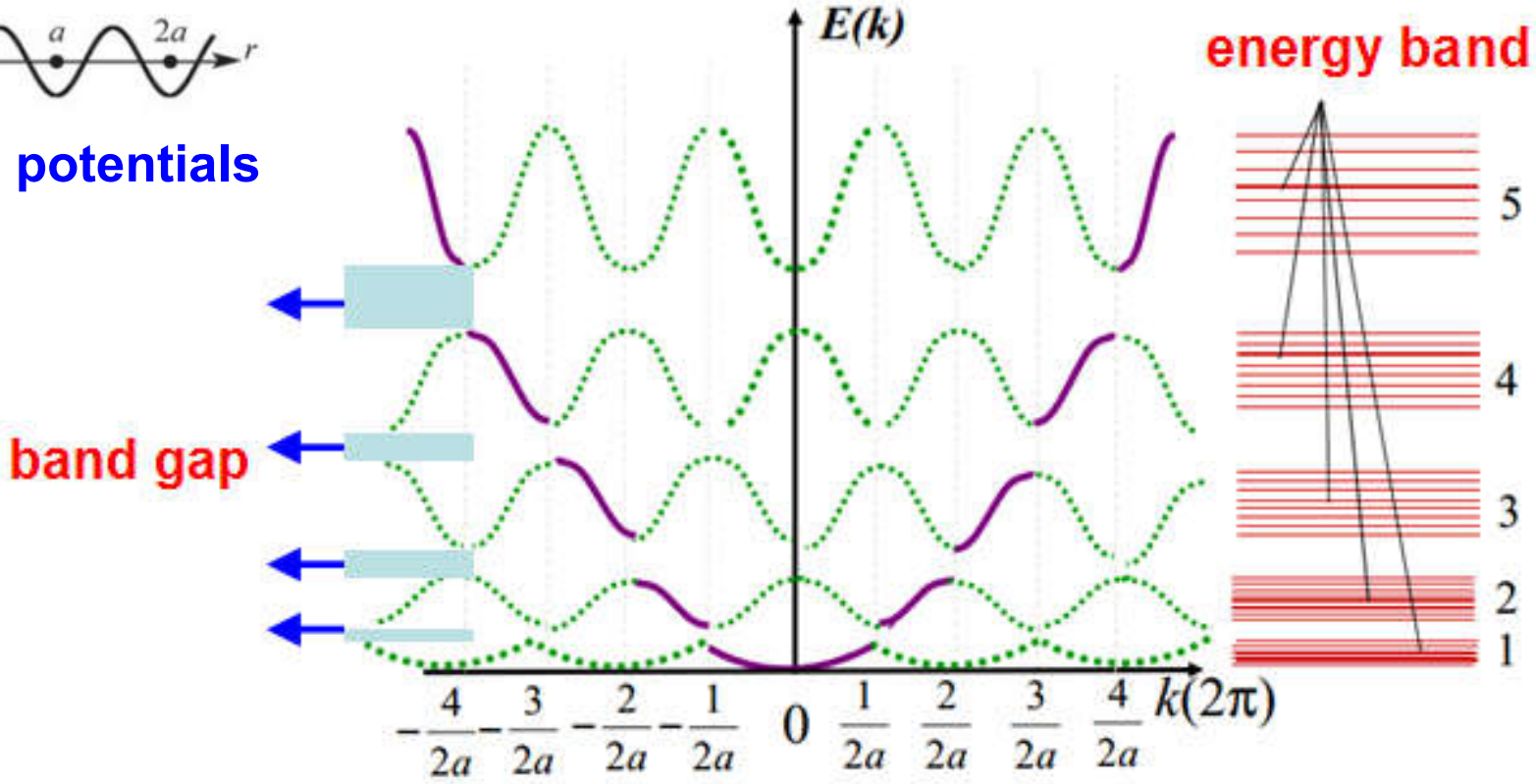

free electrons
nearly free electron model
general Bloch waves
tight binding model
isolated atoms
$V(x)$
$V(\mathbf{r}) = 0$
E
k_x
$\psi(\mathbf{r}) \sim \exp(i\mathbf{k} \cdot \mathbf{r})$

Summary

free electrons | nearly free electron model | general Bloch waves | tight binding model | isolated atoms $V(x)$



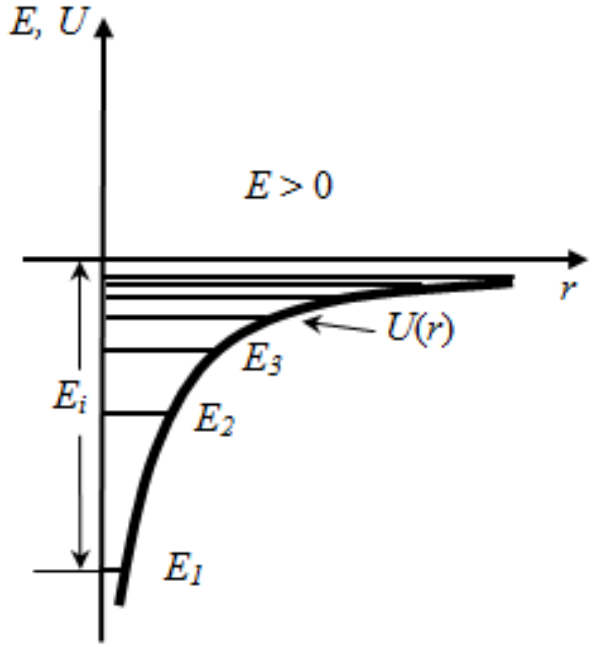
weak, periodic potentials



Summary

free electrons → nearly free electron model → general Bloch waves → tight binding model → isolated atoms → $V(x)$

hydrogen atom

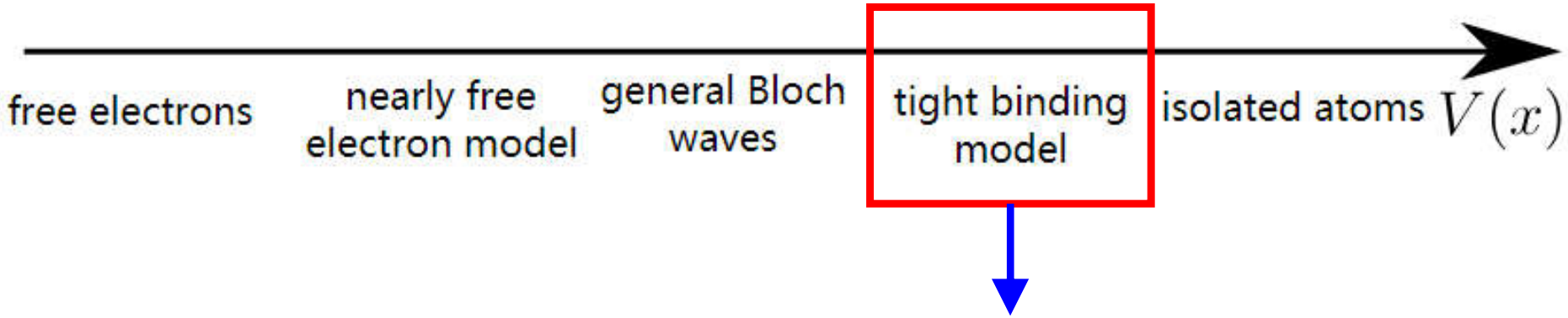


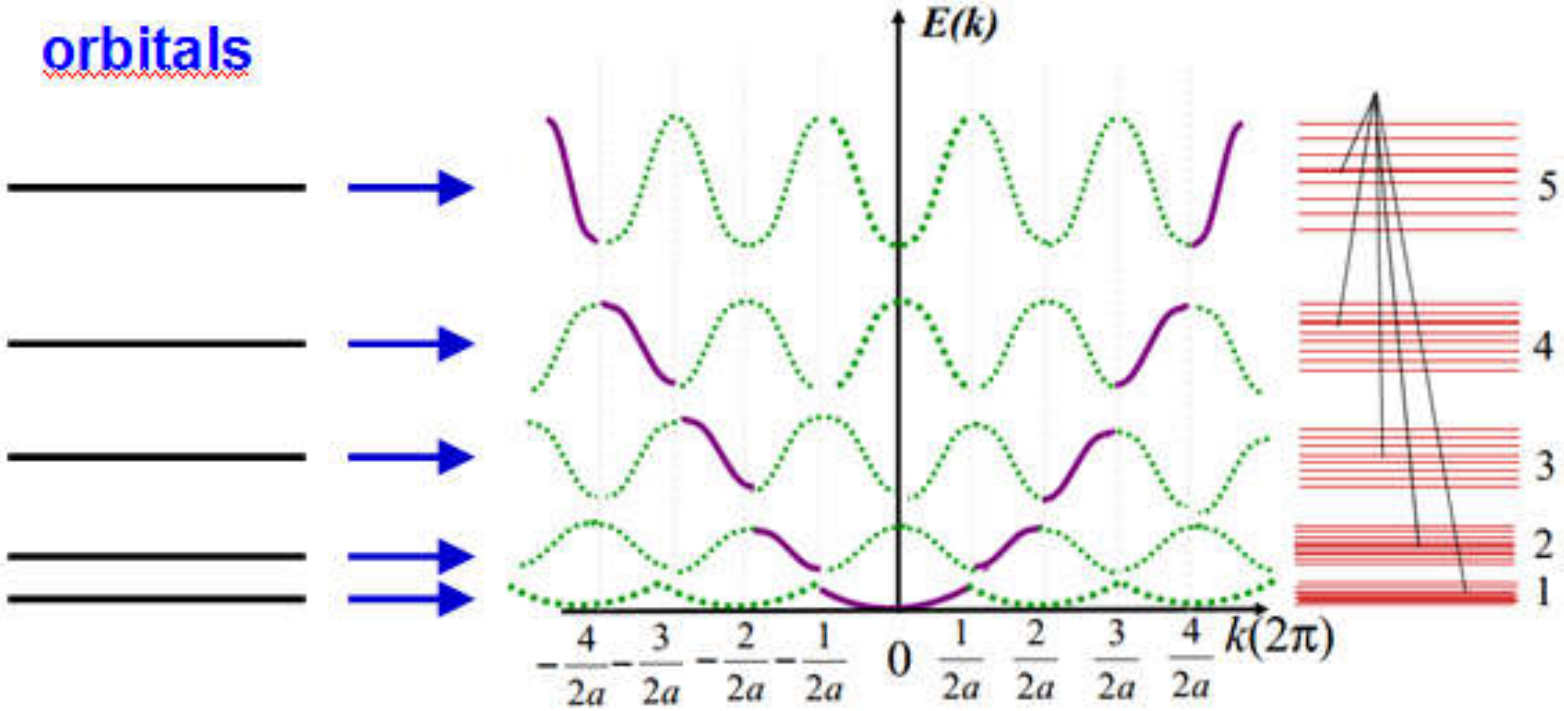
$$V(\mathbf{r}) = -\frac{e^2}{4\pi\varepsilon_0}\frac{1}{\mathbf{r}}$$

$$E_n = -\frac{13.6\,\text{eV}}{n^2}$$

$$\psi(r,\theta,\varphi) = R_{nl}(r)\cdot Y_{lm}(\theta,\varphi)$$

Summary



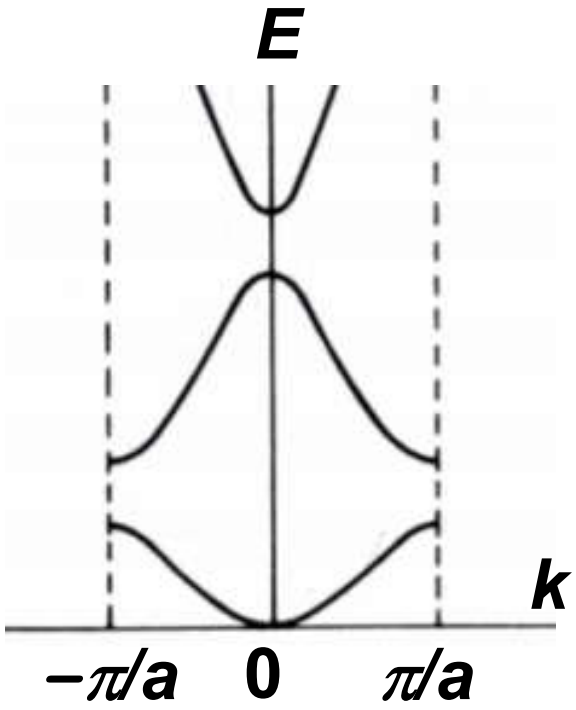


band structures and band gaps

Importance of k

- k is taken from reciprocal space
  - reduced to FBZ

$$k_x = \frac{2\pi n_x}{L_x} \qquad n_x = 0, \pm 1, \pm 2, \ldots$$



- $p = \hbar k$ is not electron momentum, is crystal momentum (take the crystal as a whole)

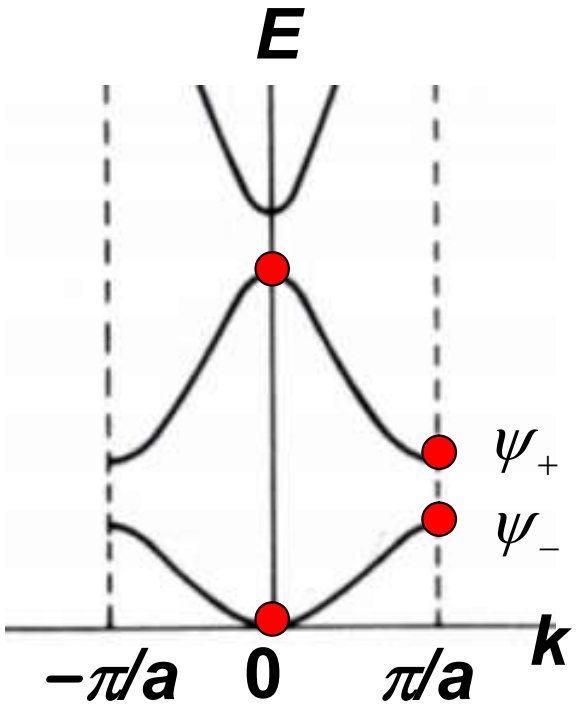
- group velocity
  - velocity of a wave packet (波包)

$$v_g = \frac{1}{\hbar}\frac{dE(k)}{dk} \quad \text{or} \quad \mathbf{v}_g = \frac{1}{\hbar}\nabla_{\mathbf{k}} E(\mathbf{k})$$

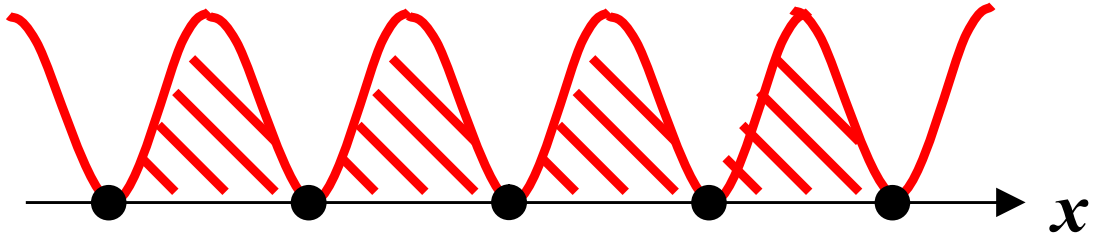
Group Velocity

- At the top and the bottom of the energy bands, $v_g = 0$
  - standing waves

$$v_g = \frac{1}{\hbar}\frac{dE(k)}{dk}$$



$$|\psi_+|^2 \sim \sin^2(\pi x / a)$$



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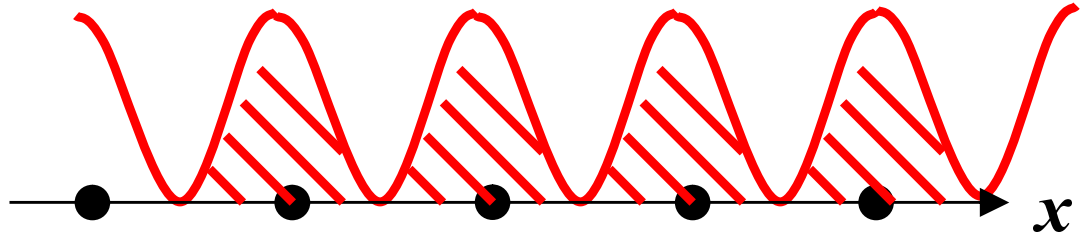


Sommerfeld vs. Bloch

	SOMMERFELD	BLOCH
QUANTUM NUMBERS (EXCLUDING SPIN)	$\mathbf{k}$ ($\hbar\mathbf{k}$ is the momentum.)	$\mathbf{k}$, n ($\hbar\mathbf{k}$ is the crystal momentum and n is the band index.)
RANGE OF QUANTUM NUMBERS	$\mathbf{k}$ runs through all of k-space consistent with the Born-von Karman periodic boundary condition.	For each n, $\mathbf{k}$ runs through all wave vectors in a single primitive cell of the reciprocal lattice consistent with the Born-von Karman periodic boundary condition; n runs through an infinite set of discrete values.
ENERGY	$\varepsilon(\mathbf{k}) = \frac{\hbar^2 k^2}{2m}$.	For a given band index n, $\varepsilon_n(\mathbf{k})$ has no simple explicit form. The only general property is periodicity in the reciprocal lattice: $\varepsilon_n(\mathbf{k} + \mathbf{K}) = \varepsilon_n(\mathbf{k})$.
VELOCITY	The mean velocity of an electron in a level with wave vector $\mathbf{k}$ is: $\mathbf{v} = \frac{\hbar\mathbf{k}}{m} = \frac{1}{\hbar}\frac{\partial\varepsilon}{\partial\mathbf{k}}$.	The mean velocity of an electron in a level with band index n and wave vector $\mathbf{k}$ is: $\mathbf{v}_n(\mathbf{k}) = \frac{1}{\hbar}\frac{\partial\varepsilon_n(\mathbf{k})}{\partial\mathbf{k}}$.
WAVE FUNCTION	The wave function of an electron with wave vector $\mathbf{k}$ is: $\psi_{\mathbf{k}}(\mathbf{r}) = \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{V^{1/2}}$.	The wave function of an electron with band index n and wave vector $\mathbf{k}$ is: $\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_{n\mathbf{k}}(\mathbf{r})$ where the function $u_{n\mathbf{k}}$ has no simple explicit form. The only general property is periodicity in the direct lattice: $u_{n\mathbf{k}}(\mathbf{r} + \mathbf{R}) = u_{n\mathbf{k}}(\mathbf{r})$.

Ashcroft & Mermin p.214

Semi-Classical Model

- **Electrons are described as wave packets (波包)**

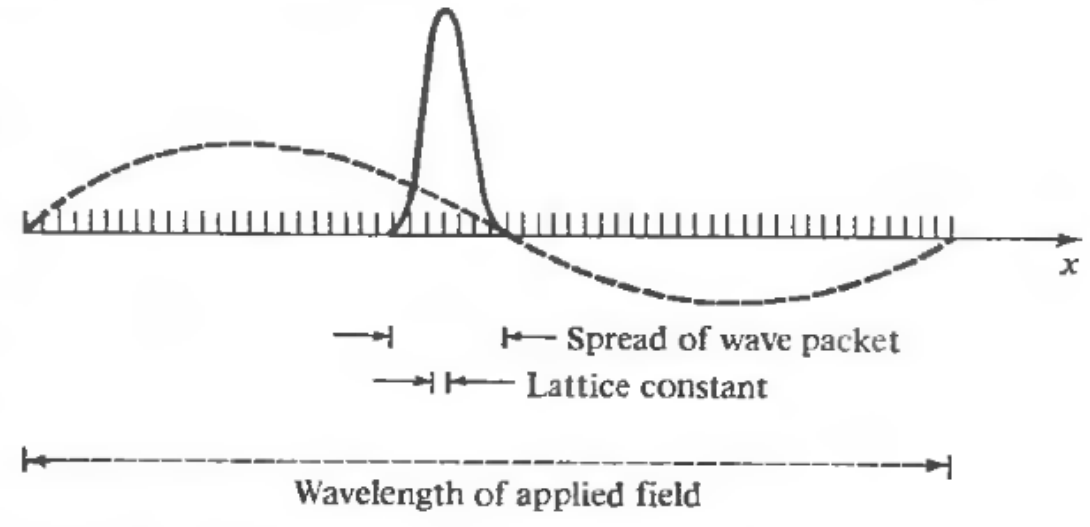
$$\psi(\mathbf{r}) = \exp(i\mathbf{k}\cdot\mathbf{r})\cdot u_{\mathbf{k}}(\mathbf{r})$$

- **Uncertainty principle**

Ashcroft & Mermin, Chap. 12

  - **wave packets spread over many cells**

$$\Delta x \cdot \Delta p \geq \hbar/2 \quad \rightarrow \quad \Delta x \cdot \Delta k \geq 1/2 \quad \rightarrow \quad \Delta x > na$$



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$$\Delta x \cdot \Delta p \geq \hbar/2 \quad \rightarrow \quad \Delta x \cdot \Delta k \geq 1/2 \quad \rightarrow \quad \Delta x > na$$

- External electric field varies slowly (DC or AC)

$$\lambda \gg a$$

- Collision / relaxation time τ
  - originates from imperfect lattice (vibrations, impurities, defects, etc.), not from single atoms
  - mean free path $l = v_F \tau \gg a$

Semi-Classical Model

$$F = \frac{dp}{dt} = \hbar \frac{dk}{dt}$$

$$v = \frac{1}{\hbar}\frac{dE}{dk} \rightarrow a = \frac{dv}{dt} = \frac{1}{\hbar}\frac{d^2E}{dk \cdot dt}$$

$$\rightarrow \frac{F}{a} = \frac{\hbar^2}{\dfrac{d^2E}{dk^2}} = m^*$$

effective mass

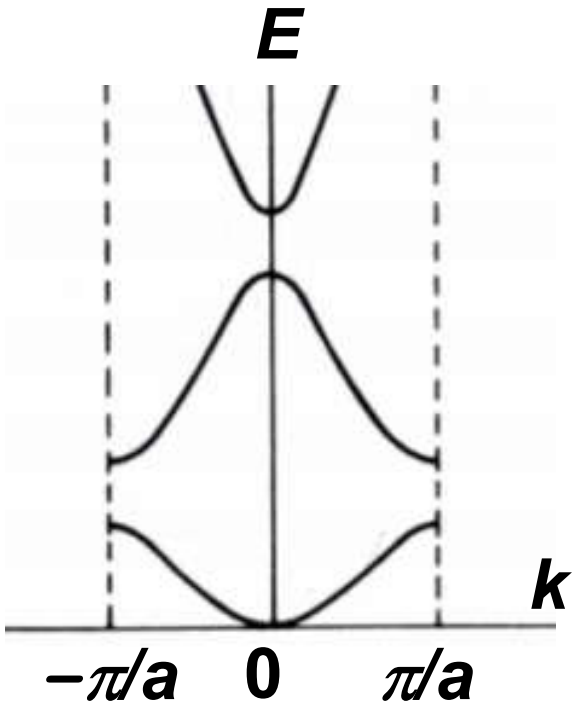
3D

$$\frac{1}{\hbar^2}\begin{pmatrix} \frac{\partial^2 E}{\partial k_x^2} & \frac{\partial^2 E}{\partial k_x \partial k_y} & \frac{\partial^2 E}{\partial k_x \partial k_z} \\ \frac{\partial^2 E}{\partial k_y \partial k_x} & \frac{\partial^2 E}{\partial k_y^2} & \frac{\partial^2 E}{\partial k_y \partial k_z} \\ \frac{\partial^2 E}{\partial k_z \partial k_x} & \frac{\partial^2 E}{\partial k_z \partial k_y} & \frac{\partial^2 E}{\partial k_z^2} \end{pmatrix} \begin{pmatrix} F_x \\ F_y \\ F_z \end{pmatrix} = \begin{pmatrix} \frac{dv_x}{dt} \\ \frac{dv_y}{dt} \\ \frac{dv_z}{dt} \end{pmatrix}$$

Effective Mass 有效质量

effective mass

$$\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{d^2E(k)}{dk^2}$$



The mass that an electron "seems" to have in a solid. It has nothing to do with the free electron mass m_0

For 3D solids, a tensor form

$$\frac{1}{\mathbf{M}^*} = \frac{1}{\hbar^2}\begin{pmatrix} \frac{\partial^2 E}{\partial k_x^2} & \frac{\partial^2 E}{\partial k_x \partial k_y} & \frac{\partial^2 E}{\partial k_x \partial k_z} \\ \frac{\partial^2 E}{\partial k_y \partial k_x} & \frac{\partial^2 E}{\partial k_y^2} & \frac{\partial^2 E}{\partial k_y \partial k_z} \\ \frac{\partial^2 E}{\partial k_z \partial k_x} & \frac{\partial^2 E}{\partial k_z \partial k_y} & \frac{\partial^2 E}{\partial k_z^2} \end{pmatrix}$$

m^* is a function of k, can be smaller or larger than m_0, even can be negative

$m_0 = 9.11*10^{-31}$ kg

Effective Mass 有效质量

effective mass

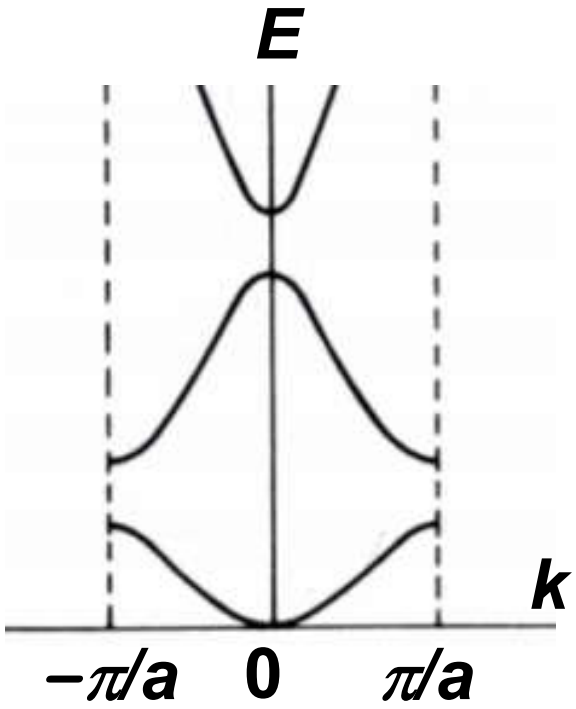
$$\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{d^2E(k)}{dk^2}$$

mobility

$$\mu = \frac{v}{E} = e\frac{\tau}{m^*}$$

conductivity

$$\sigma = ne\mu = ne^2\frac{\tau}{m^*}$$



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effective mass

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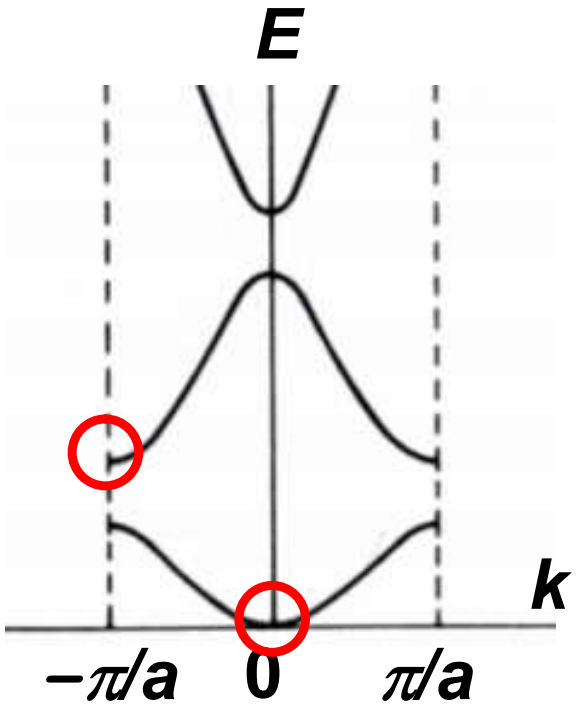


close to band minimum
parabolic approximation

$$E(k) \approx E_0 + \frac{\hbar^2}{2m^*}(k-k_0)^2$$

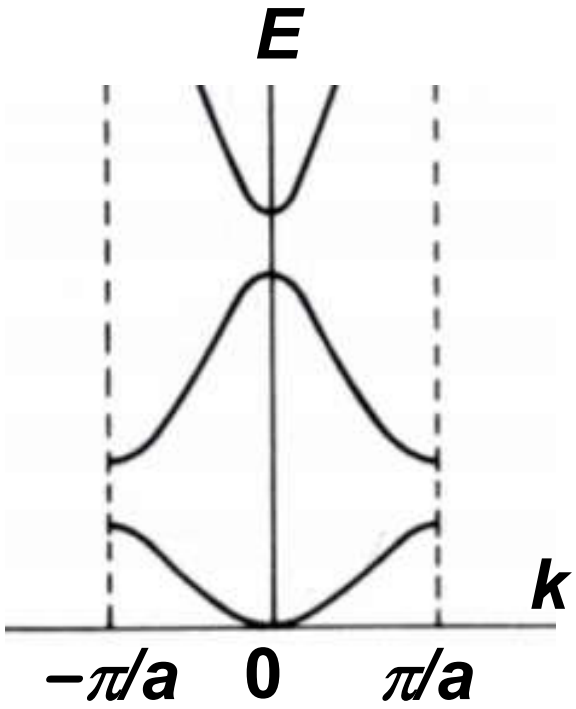
3D DOS

$$g(E) = \frac{dn}{dE} = \frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}(E-E_0)^{1/2}$$

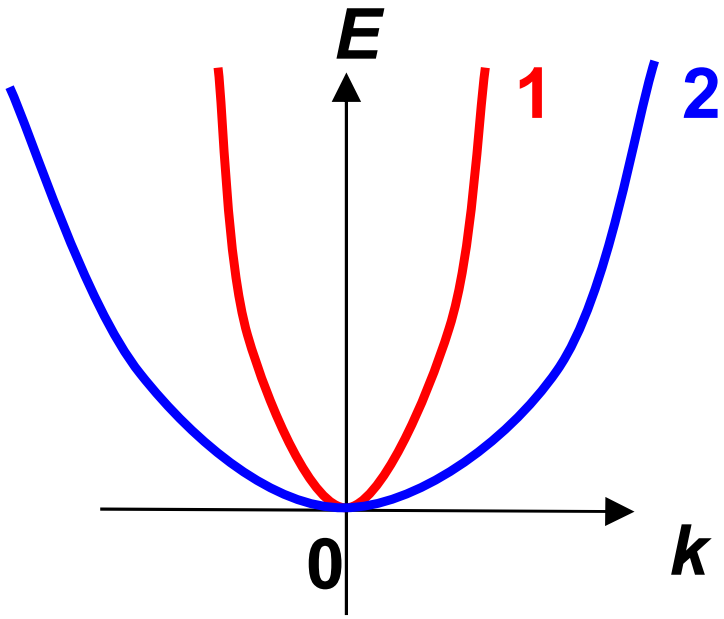
Effective Mass 有效质量

effective mass

$$\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{d^2E(k)}{dk^2}$$



inverse curvature of the parabolic curve

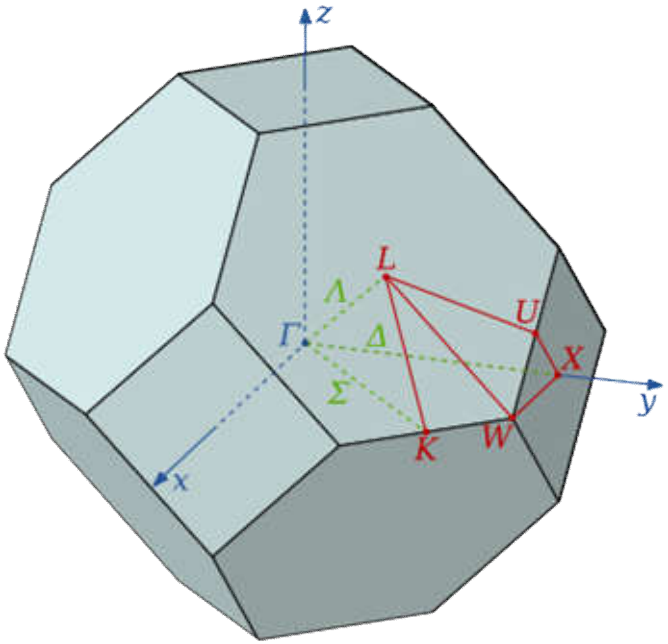


Q: $m_1 > m_2$
or $m_1 < m_2$?

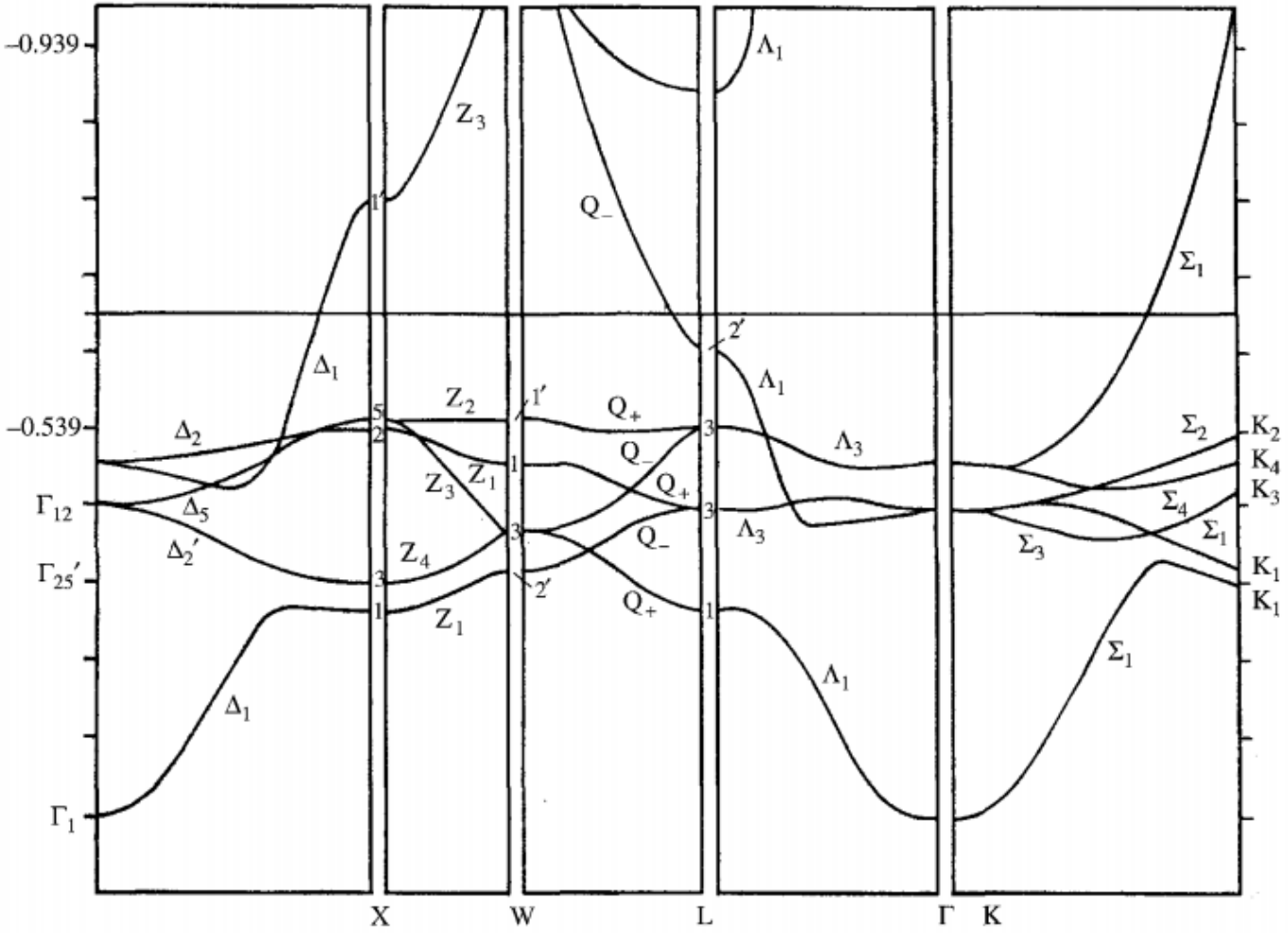
Band Structure in 3D

copper (FCC)

$$E = E(k_x, k_y, k_z)$$



First BZ

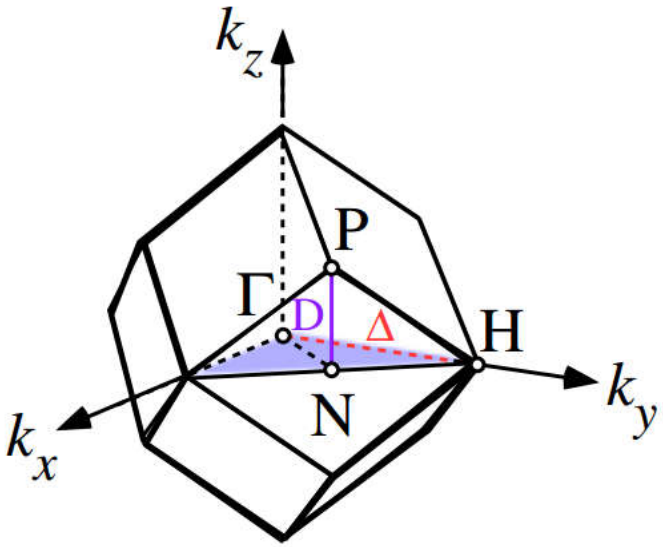


G. A. Burdick, *Phys. Rev.* **129,** 138 (1963)

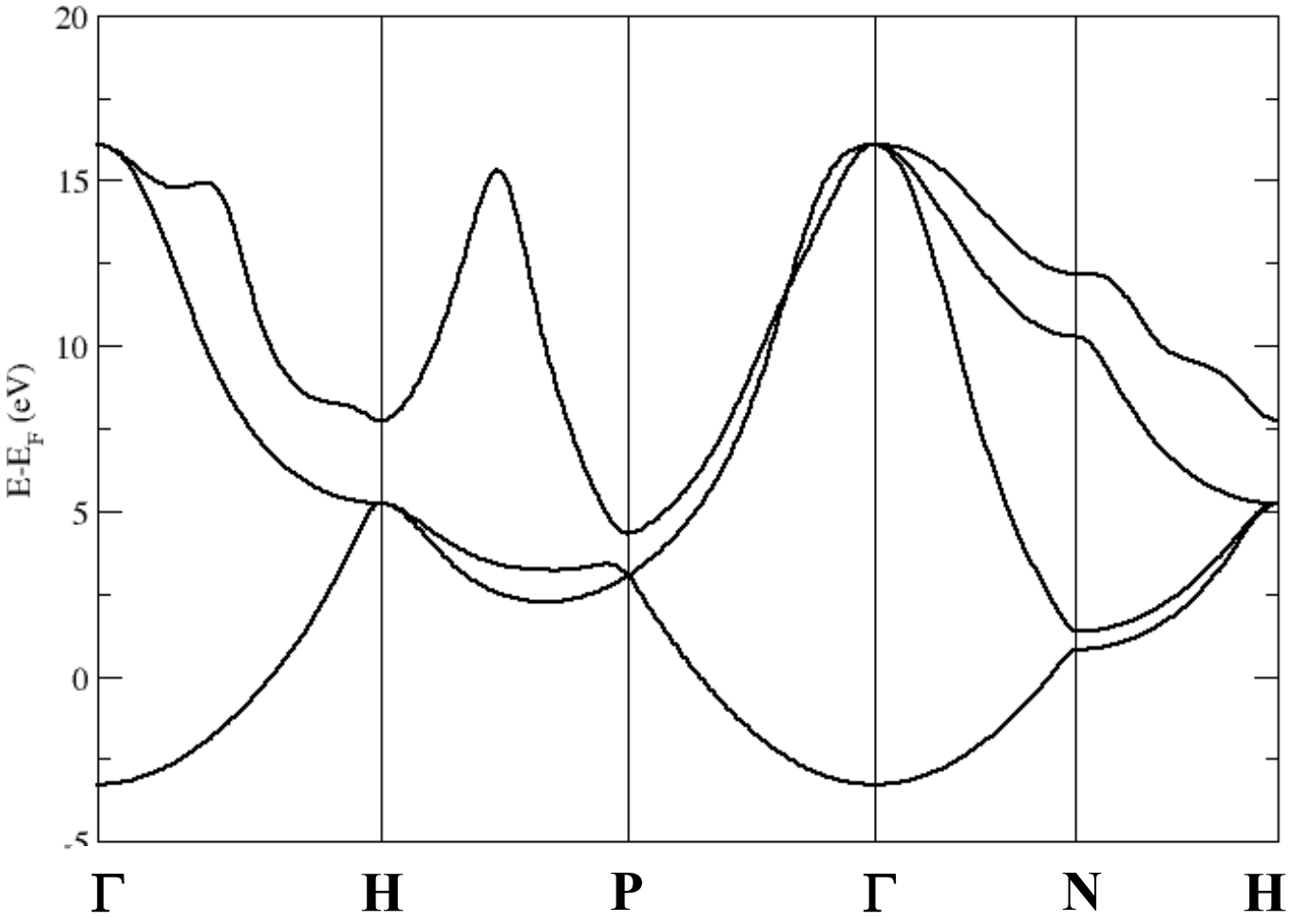
Band Structure in 3D

sodium (BCC)

$$E = E(k_x, k_y, k_z)$$



First BZ



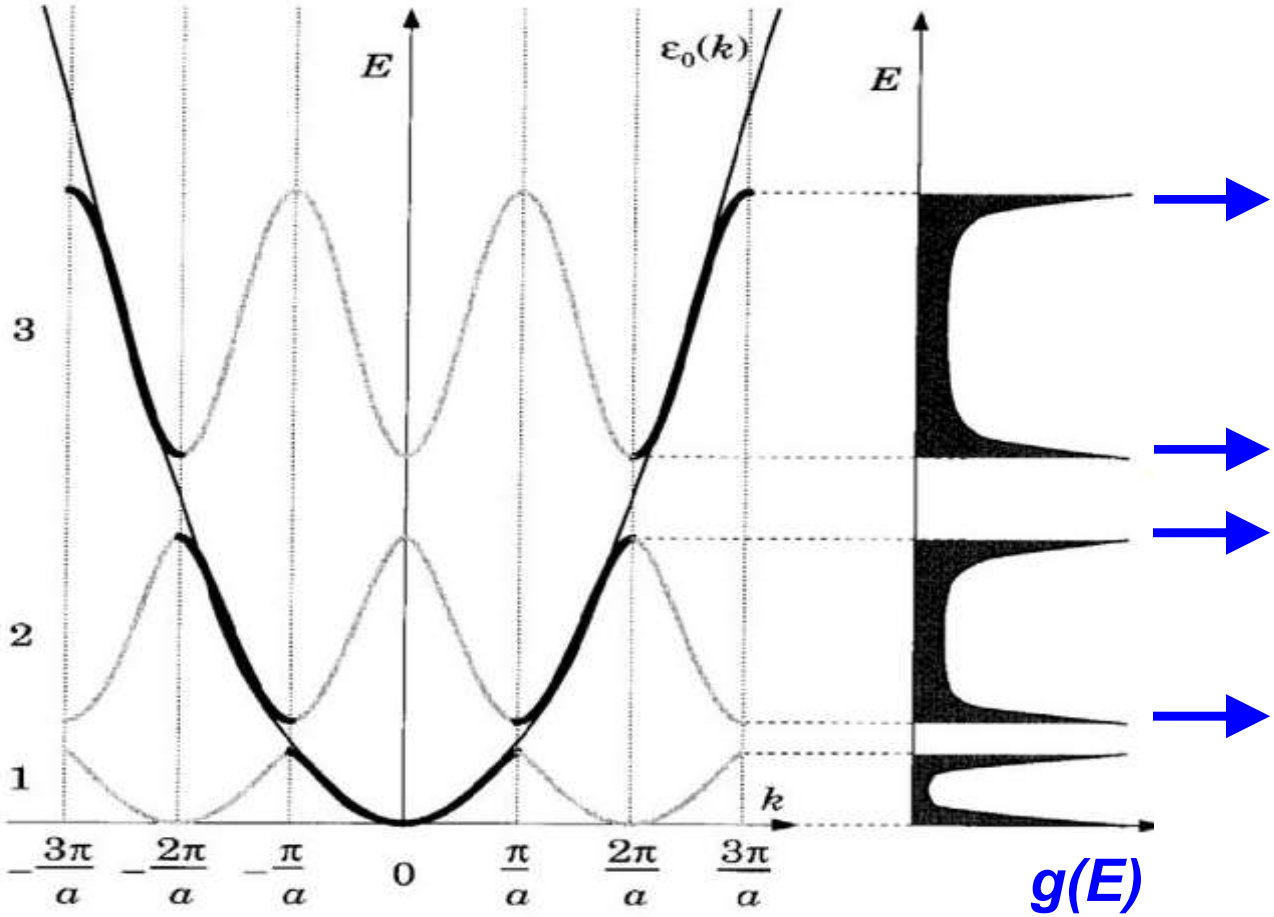
http://dipc.ehu.es/frederiksen/inelastica/index.php/Na_BCC

Density of States (DOS) 态密度

$$g(E) = \frac{dn}{dE}$$

DOS - number of energy states/levels per unit energy in [*E*, *E*+*dE*], per unit volume

1D



van Hove singularities

Density of States (DOS) 态密度

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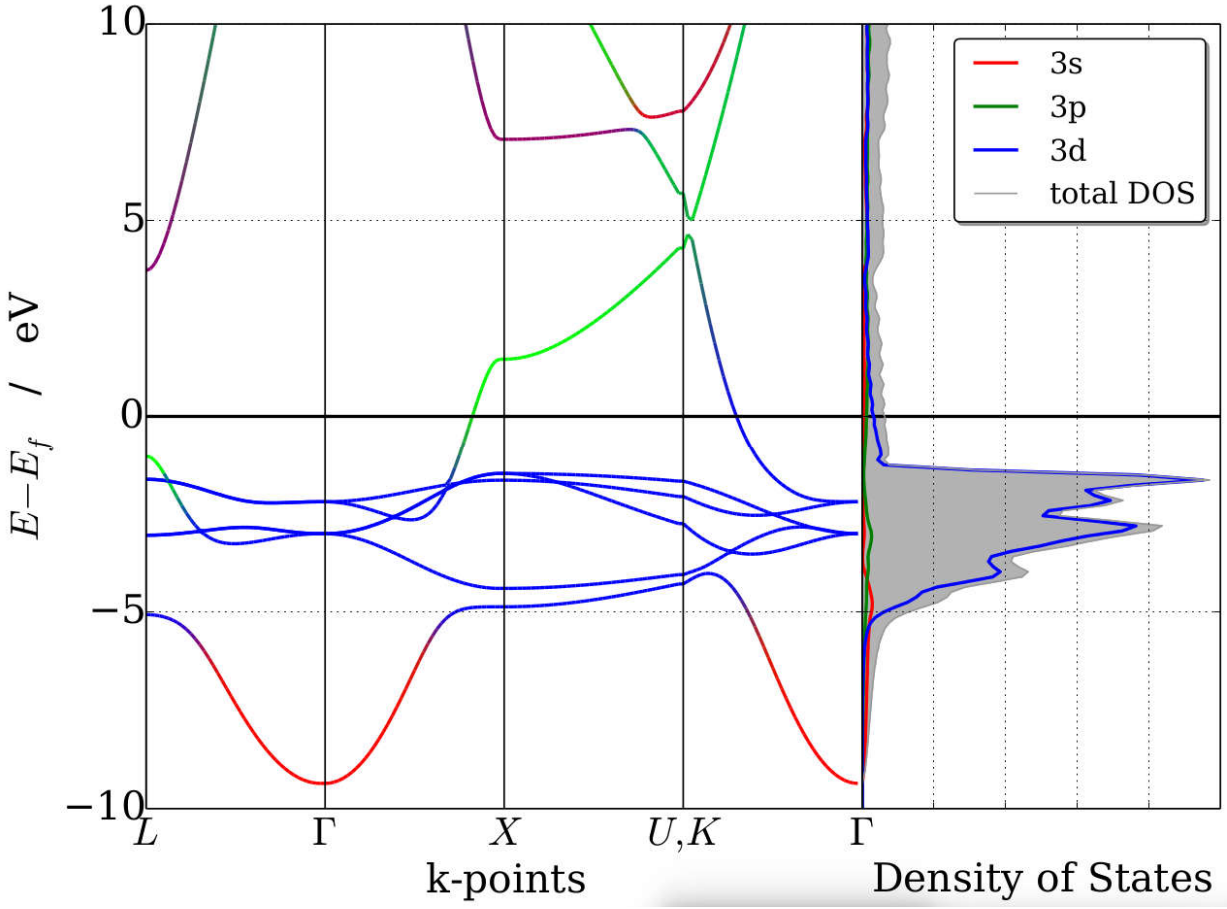
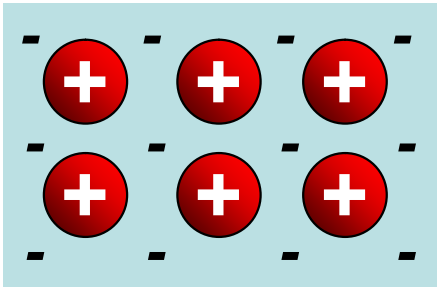
3D copper



g(E)

Bloch Model - Review

- Electrons are *not free*, but *in a periodic potential* formed by the atomic lattice



positive ions
+
electron cloud

- Born-Oppenheimer Approximation
  - The behaviors of electrons and nuclei can be calculated separately.

- Independent Electron Approximation
  - We still assume electrons are independent and do not interact with each other

Real Electrons in Solids is a Nightmare

$$\hat{H}\Psi = E\Psi$$

many-body problem '多体'问题

$$\sum_{i=1}^{N}\left(-\frac{\hbar^2}{2m}\nabla_i^2\Psi - Ze^2\sum_{\mathbf{R}}\frac{1}{|\mathbf{r}_i-\mathbf{R}|}\Psi\right)+\frac{1}{2}\sum_{i\neq j}\frac{e^2}{|\mathbf{r}_i-\mathbf{r}_j|}\Psi = E\Psi$$

free electron

electron-atom interaction

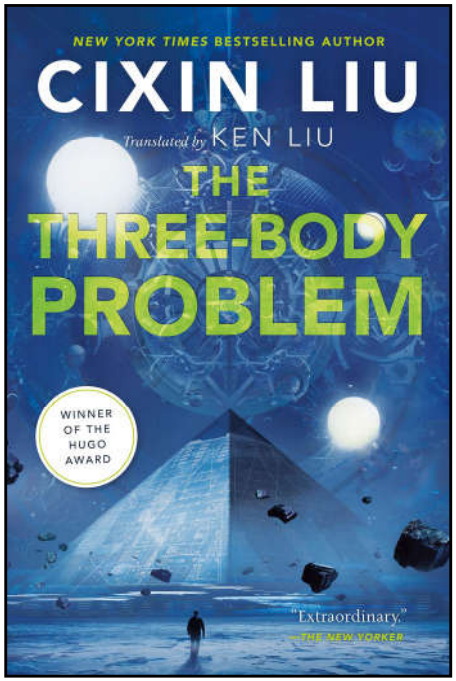
electron-electron interaction

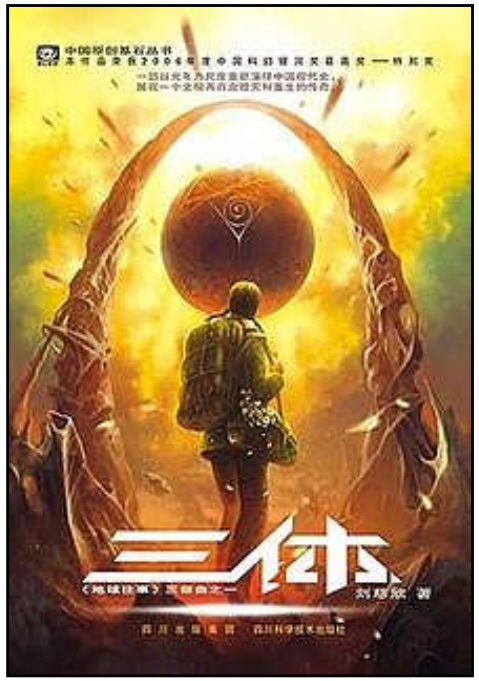
Wave function is complicated and impossible to solve

Real Electrons in Solids is a Nightmare

$$\hat{H}\Psi = E\Psi$$

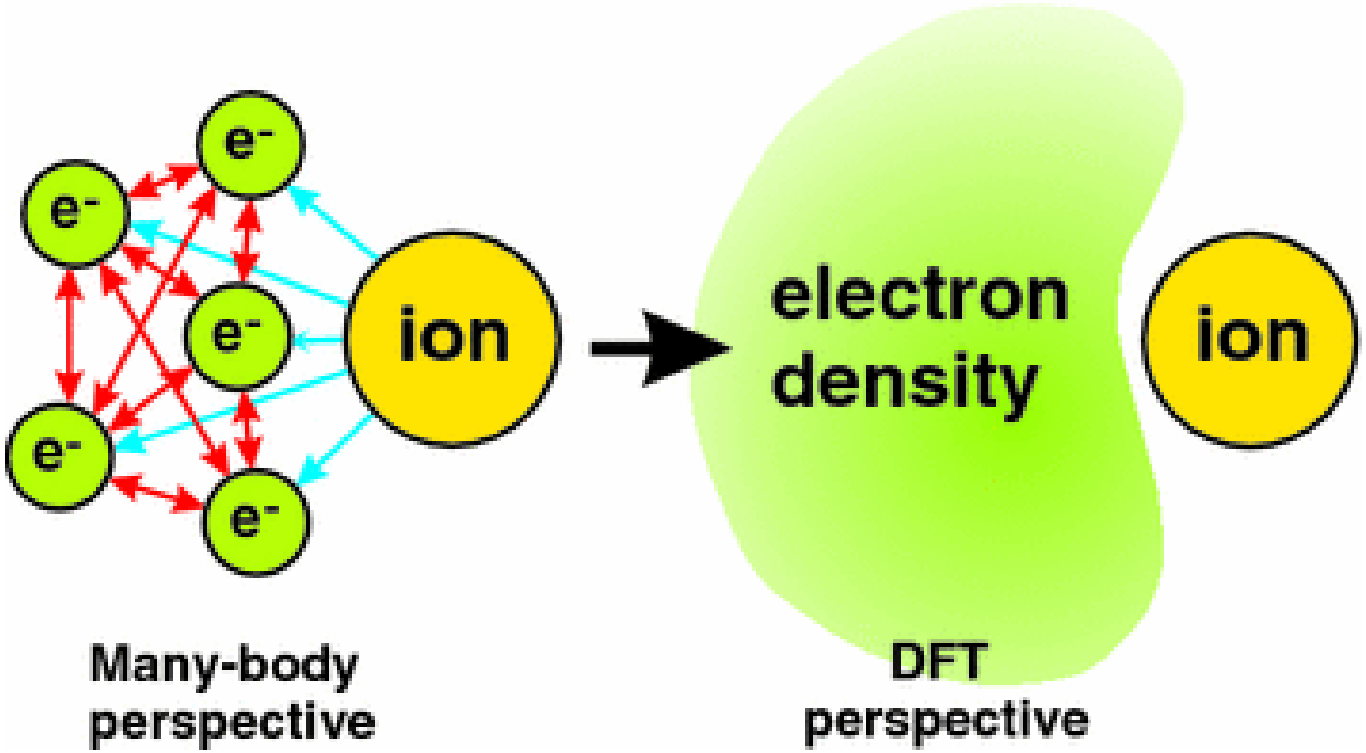
many-body problem '多体'问题





Wave function is complicated and impossible to solve

Density Functional Theory (DFT) 密度泛函理论



wave function → electron density

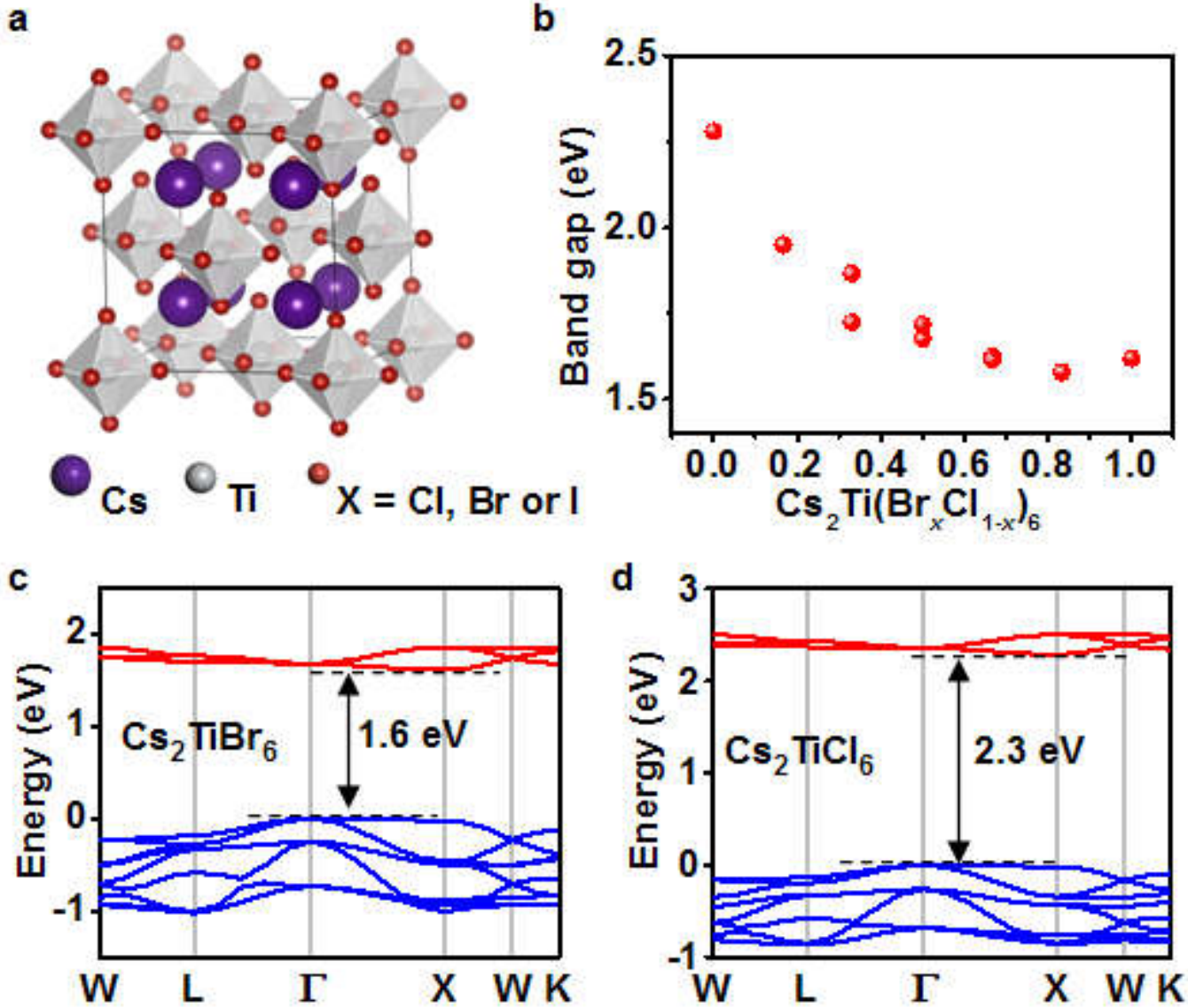
Photo from the Nobel Foundation archive.

Walter Kohn

Prize share: 1/2

Nobel Prize in Chemistry 1998

Band Structures by DFT - Example

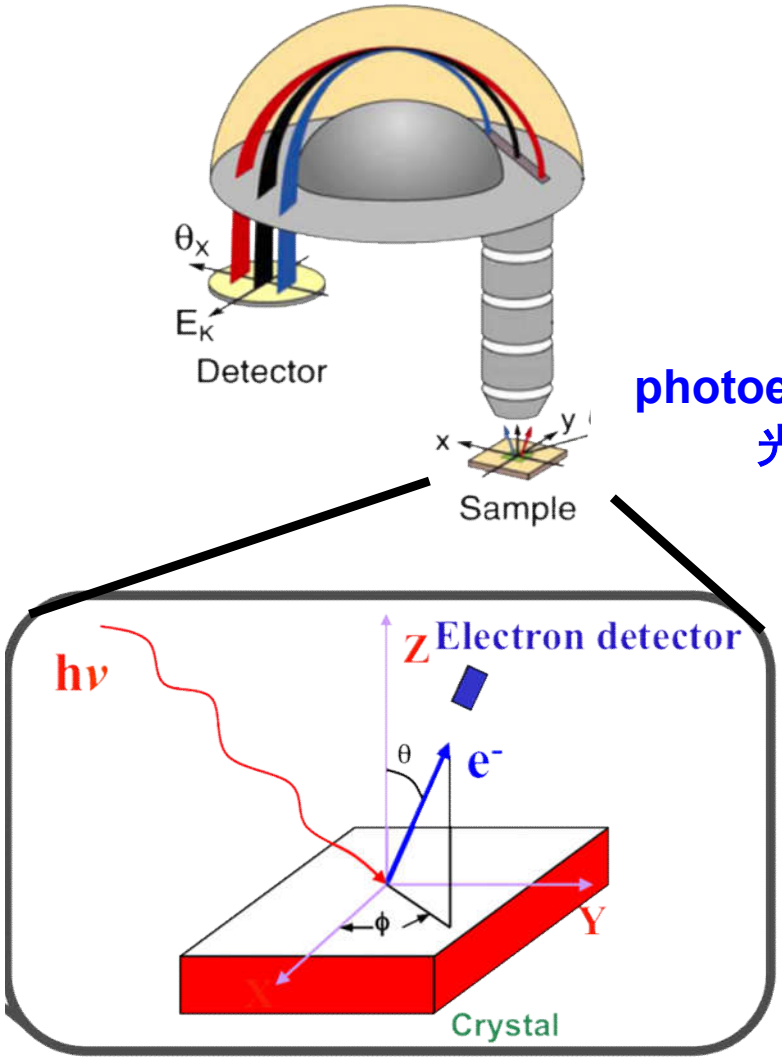


work by 2016级本科生 成大立

D. Kong, *et al*, *J. Mater. Chem. C* **8,** 1591 (2020)

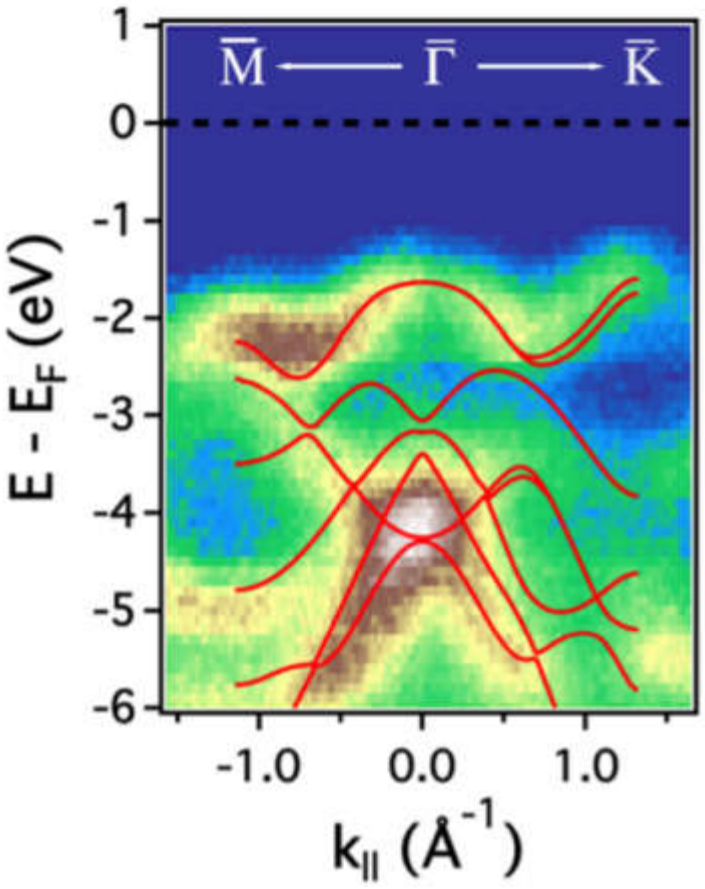
Measurement of Band Structures

Angle-Resolved Photoemission Spectroscopy (ARPES)



photoelectric effect
光电效应

MoS_2



W. Jin, *et al*, *Phys. Rev. Lett.* **111,** 106801 (2013)

https://arpes.stanford.edu/research/tool-development/angle-resolved-photoemission-spectroscopy

Thank you for your attention