Condensed Matter Physics I

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Previously

- Free electron model
- Density of states, Fermi-Dirac distribution
- Pressure, Bulk modulus, Heat capacity, Thermal mass
- Charge conductivity
- Classical Hall effect
- Electronic thermal transport, Wiedemann-Franz
- Failures of free e- model
- Incorporation periodic potential, Bloch states, gaps

Today

-

Band structure: Approaches

- Empty lattice (only periodicity)
- Perturbation theory (nearly free electrons, weak potential)
- Tight binding method (LCAO)
- Exact models (Kronig-Penney model, see for instance Kittel)
- ‘advanced’ methods: see for instance
  ashcroft and mermin, chapter 11

Diamond band structure

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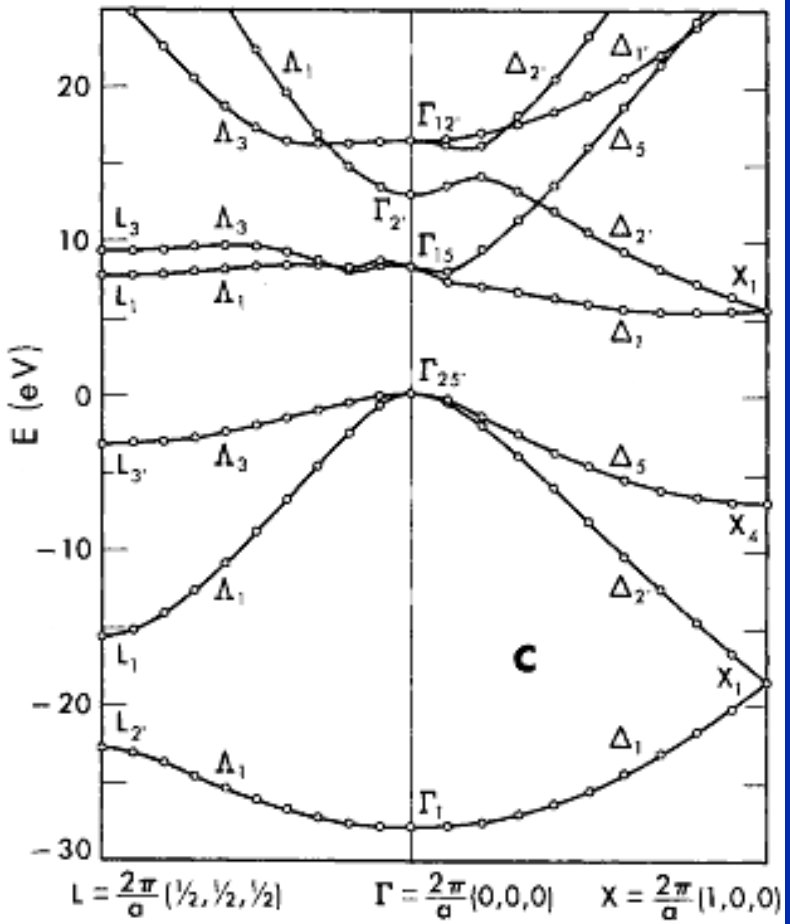

FIG. 1. The electronic band structure of diamond.

BAND STRUCTURE AND OPTICAL PROPERTIES OF DIAMOND*

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(Received 27 January 1966)

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Electronic band structure of the superconductor Sr_2RuO_4

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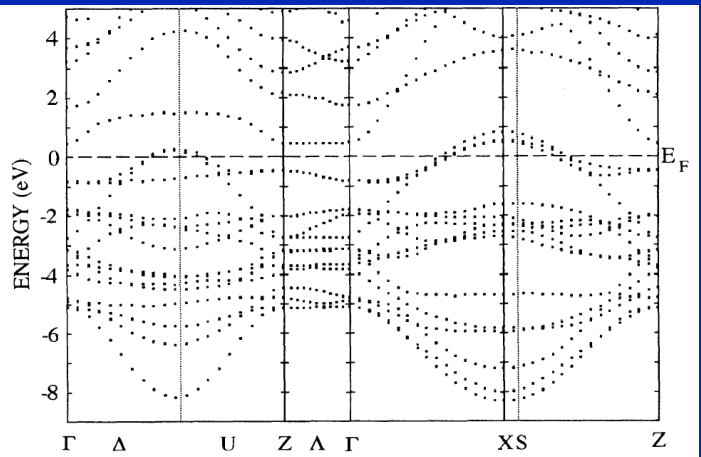


FIG. 1. Calculated energy band structure of Sr_2RuO_4 along high-symmetry lines. A horizontal broken line denotes the Fermi energy.

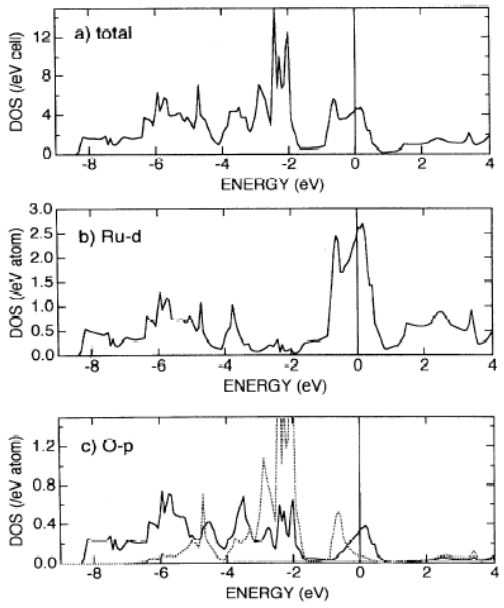


FIG. 3. Calculated density of states (DOS) of Sr_2RuO_4: (a) total DOS, (b) partial Ru d DOS, and (c) partial O p DOS. In panel (c), solid and dotted curves represent the partial p DOS of the O(I) and O(II) atoms, respectively. A vertical line denotes the Fermi energy.

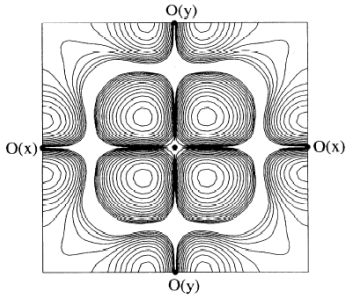
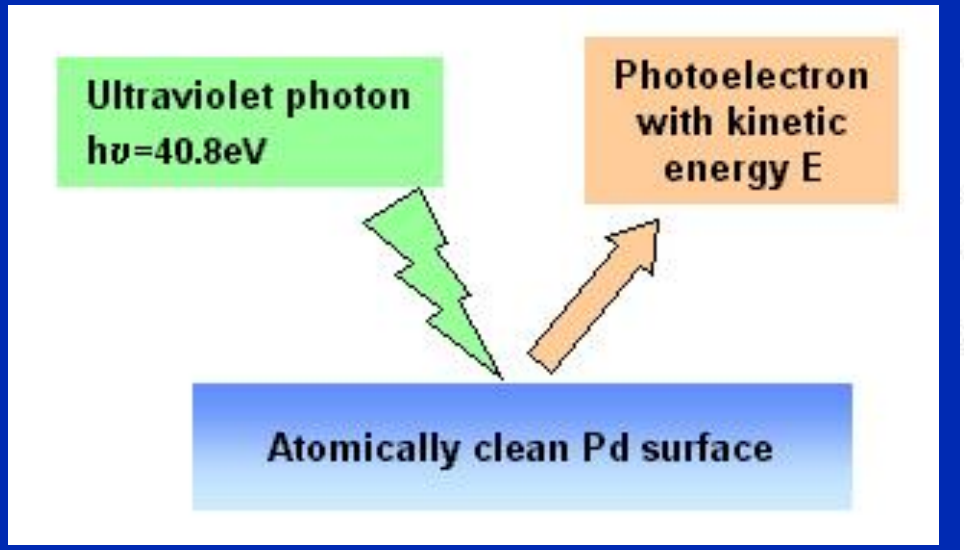


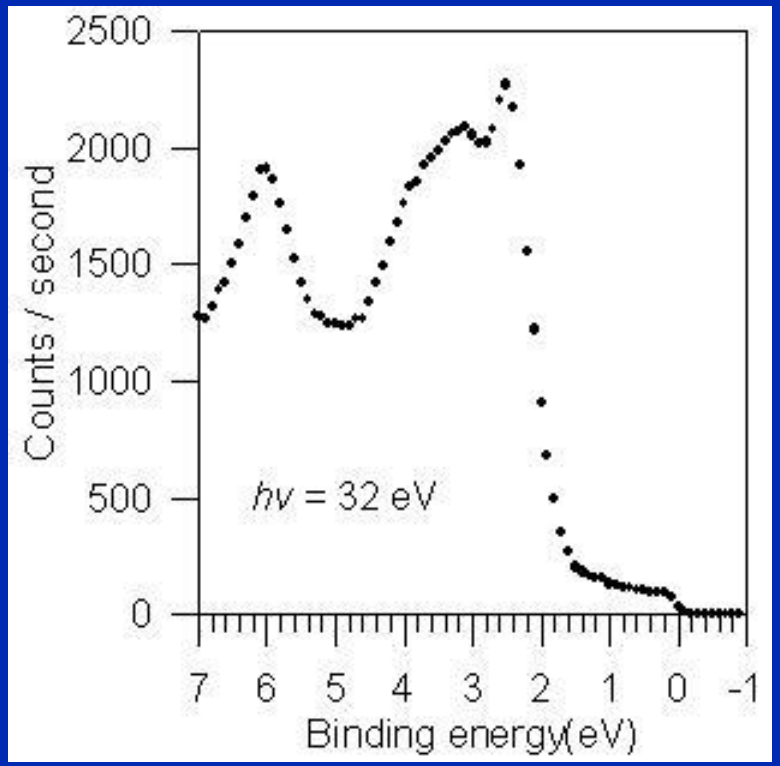
FIG. 2. An ab-plane contour map of the pseudocharge density of the antibonding $d\varepsilon(xy)$-$p\pi$ band at the X point (the 15th band in Fig. 1). Contours of charge density are plotted as $(2)^{n/2}\times 10^{-3}$ electrons/bohr^3 ($n=0,1,\ldots$). A clear node (zero amplitude of the wave function) between the Ru (at center) and four O(I) atoms indicates the antibonding character of the state.

Photoemission

$$E_{bind} = \hbar\omega - E_{kin} - \phi$$

$$\hbar k_{||}^{i} = \hbar k_{||}^{f} = \sqrt{2mE_{kin}}\sin\theta$$





Gold, U. Johansson, R. Nyholm

Photoemission

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Bulk Band Gaps in Divalent Hexaborides

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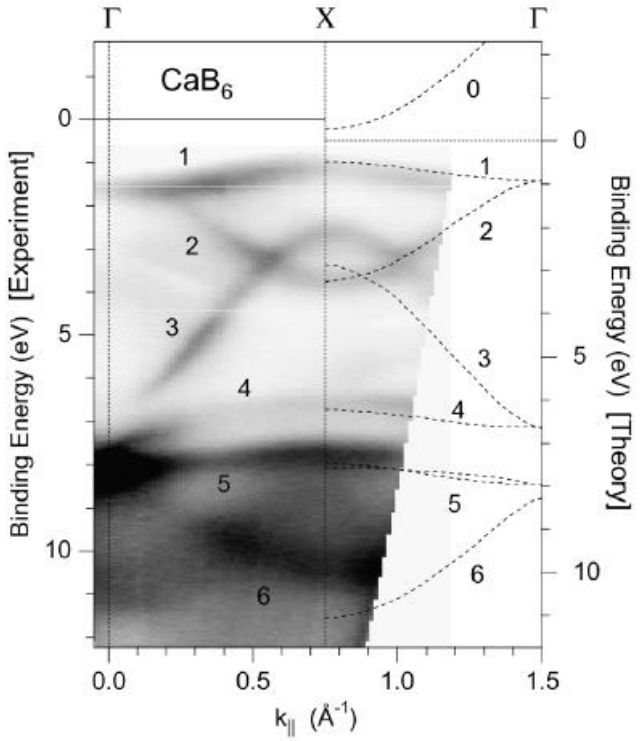
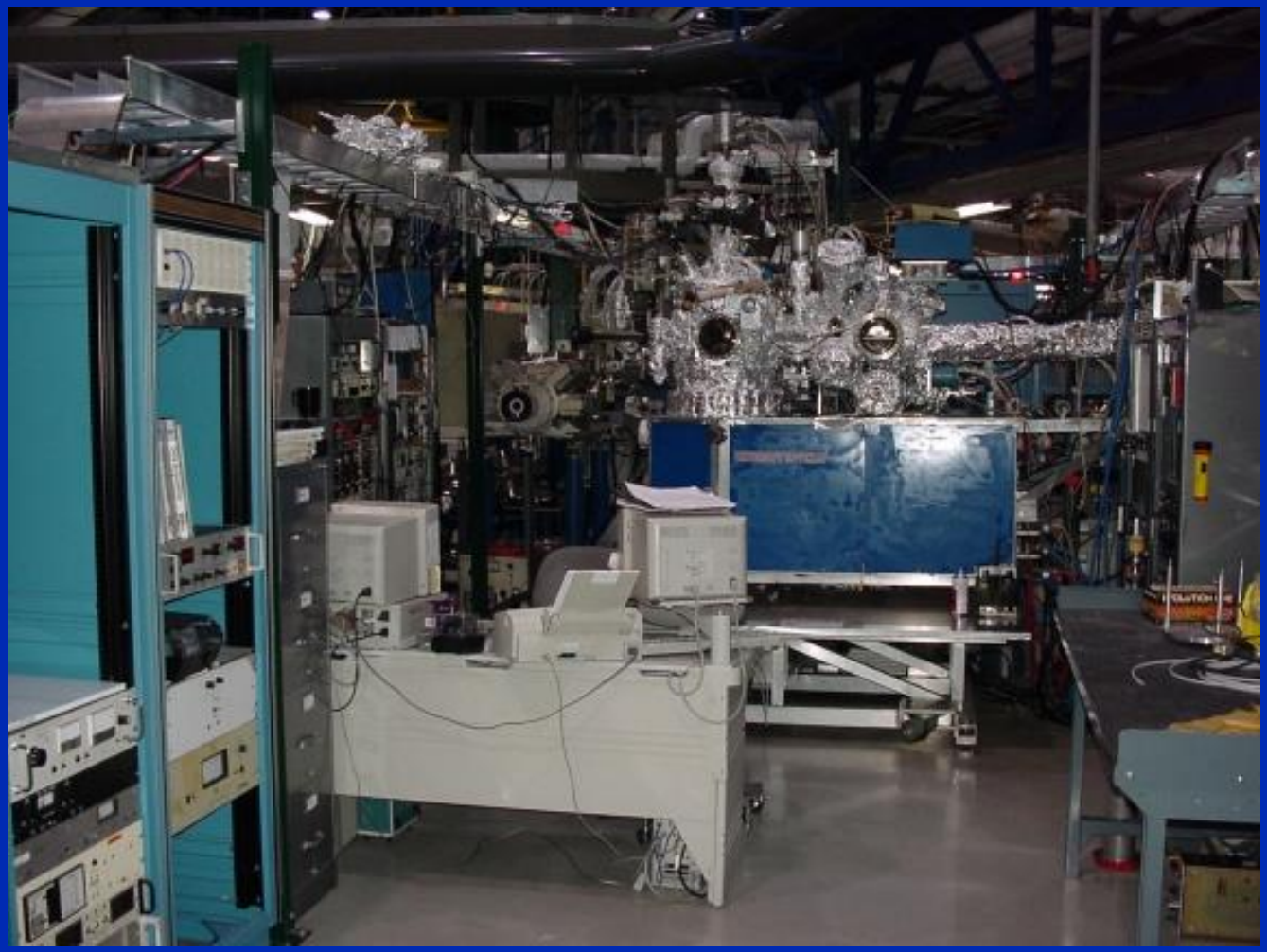


FIG. 1. Comparison of the experimental and theoretical band structures of CaB_6 along Γ-X. The reverse gray scale image of ARPES intensities is the sum of two data sets with 30 eV s- and p-polarized excitation. Dashed lines are from the quasiparticle GW calculation [18] giving X-point gap between bands 0 and 1.

Photoemission



Band Structure

Continued

Bloch theorem

Bloch Theorem

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

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

$$T_{\vec{n}} \Psi_{\vec{k}}(\vec{r}) = \Psi_{\vec{k}}(\vec{r} + \vec{R}_{\vec{n}}) = e^{i\vec{k}\cdot\vec{R}} \Psi_{\vec{k}}$$

The eigenstates of a periodic one-electron Hamiltonian can be chosen to have the form of a plane wave times a function with the periodicity of the Hamiltonian

Remarks on Blochfunctions

1. Quantum number k: Crystal momentum

$$\frac{\hbar}{i}\nabla\Psi_k = \frac{\hbar}{i}\nabla e^{i\,k\cdot r}u_k(\vec{r}) = \hbar k\cdot\Psi_k + \frac{\hbar}{i}e^{i\,k\cdot r}\nabla u_k(\vec{r})$$

2. k may be confined to the 1st BZ (Reduced BZ)

$$\Psi_{\vec{k}+\vec{G}} = e^{i\,\vec{k}\cdot\vec{r}}\,u_{\vec{k}+\vec{G}}(\vec{r})$$

3. Band index n

Born-von Karman $\Psi(\vec{r}+p_i\cdot\vec{a}_i) = \Psi(\vec{r})$

$$u_k(\vec{r}) = \sum_{\vec{G}} C_{\vec{k}+\vec{G}}\cdot e^{i\,\vec{G}\cdot\vec{r}}$$

4. Band structure $\varepsilon_n(\vec{k})$

Band structure: Approaches

Last time

- Empty lattice (only periodicity)
- Perturbation theory (nearly free electrons, weak potential)

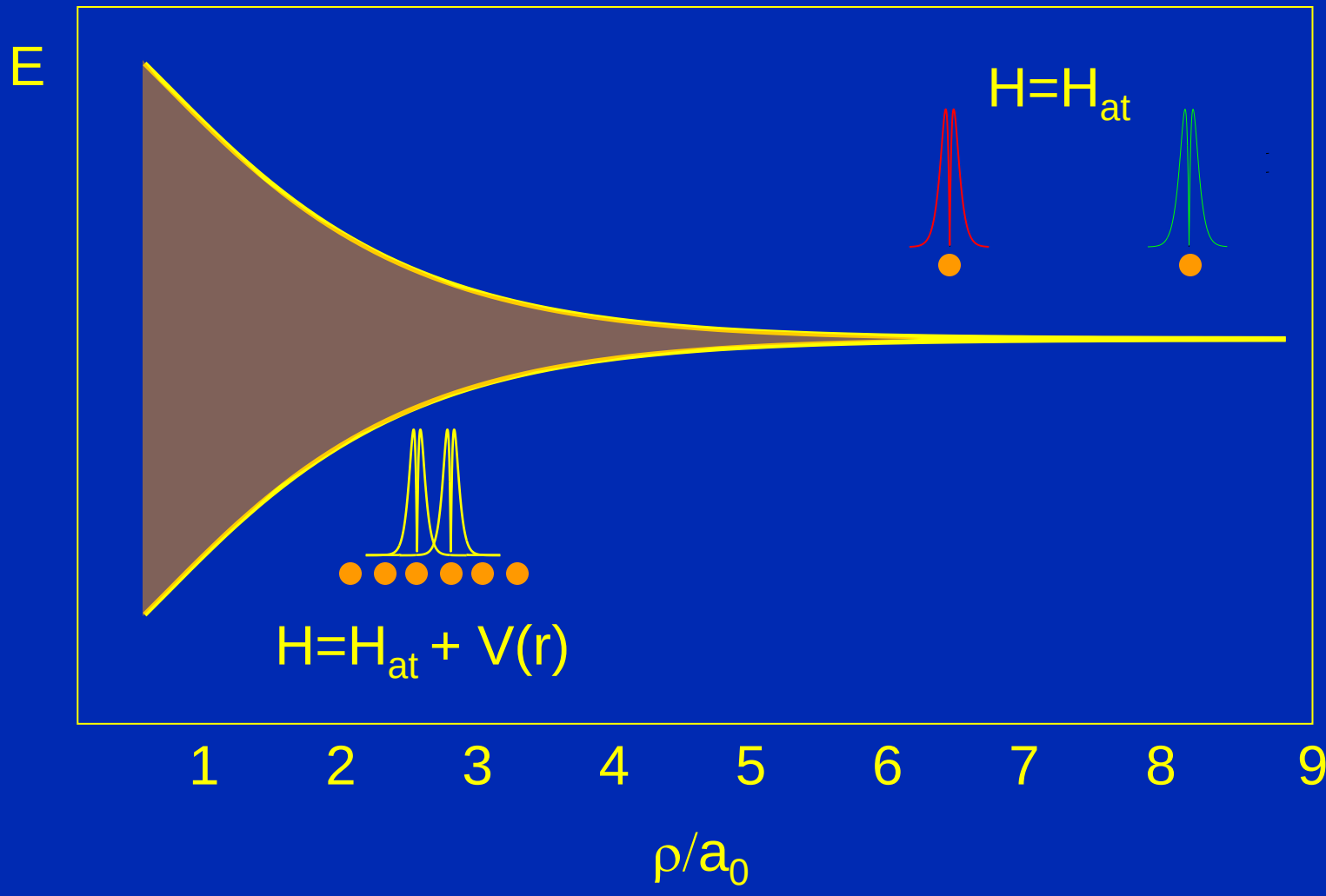
Today

- Tight binding method (LCAO)

Other methods

- Exact models (Kronig-Penney model, see book)
- ‘advanced’ methods: Ashcroft & Mermin chapter 11

Tight binding approach



Tight binding

Atomic orbitals $\varphi(r)$: $H_{at}\,\varphi(r) = E_{at}\,\varphi(r)$

Solid state: $H = H_{at} + V(r)$

$$\Rightarrow \quad \Psi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{N}} \sum_j e^{i\vec{k}\cdot\vec{r}_j} \cdot \varphi(\vec{r} - \vec{r}_j)$$

1st order correction to energy: diagonal elements

$$\langle k | H | k \rangle = \frac{1}{N} \sum_j \sum_m e^{i\vec{k}\cdot(\vec{r}_j - \vec{r}_m)} \cdot \langle \varphi_m | H | \varphi_j \rangle$$

$$= \sum_m e^{i\vec{k}\cdot\vec{\rho}_m} \cdot \int dV\ \varphi^*(\vec{r} - \vec{\rho}_m) H \varphi(\vec{r})$$

Tight binding

$$\langle k|H|k\rangle = \sum_m e^{i\vec{k}\cdot\vec{\rho}_m} \cdot \int dV\ \varphi^*(\vec{r}-\vec{\rho}_m) H \varphi(\vec{r})$$

Only nearest neighbours:

Self $\quad \rho = 0 \quad \Rightarrow \quad \int dV\ \varphi^*(\vec{r}) H \varphi(\vec{r}) \equiv -\alpha$

N.N. $\quad \rho_m = \rho \quad \Rightarrow \quad \int dV\ \varphi^*(\vec{r}-\vec{\rho}) H \varphi(\vec{r}) \equiv -\gamma$

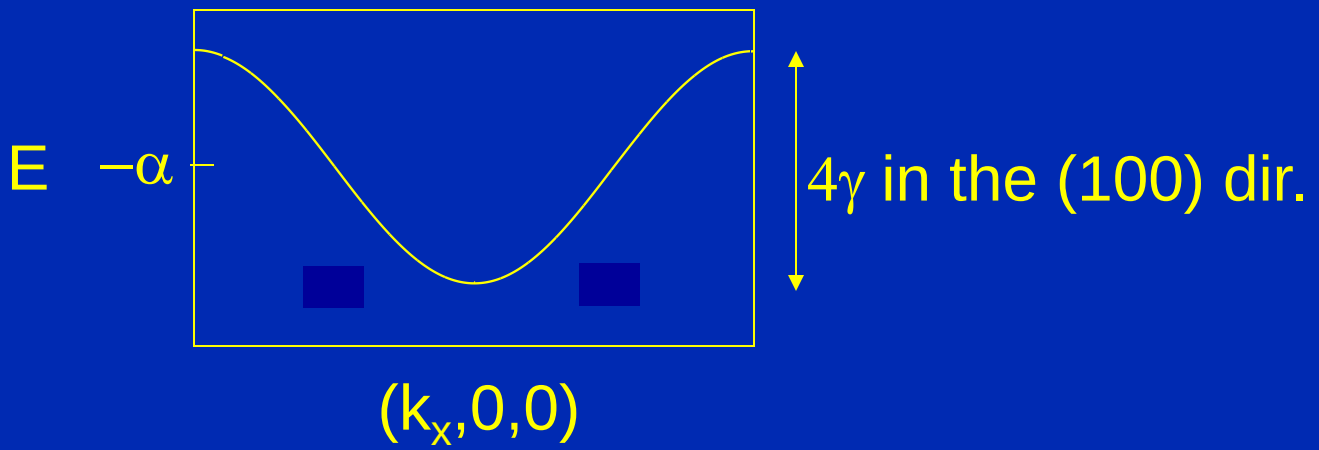
$$\varepsilon(k) = \langle k|H|k\rangle = -\alpha - \gamma \cdot \sum_{nn} e^{-i\vec{k}\cdot\vec{\rho}_{nn}}$$

Tight binding

$$\varepsilon(k) = \langle k | H | k \rangle = -\alpha - \gamma \cdot \sum_{nn} e^{-i\,\vec{k}\cdot\vec{\rho}_{nn}}$$

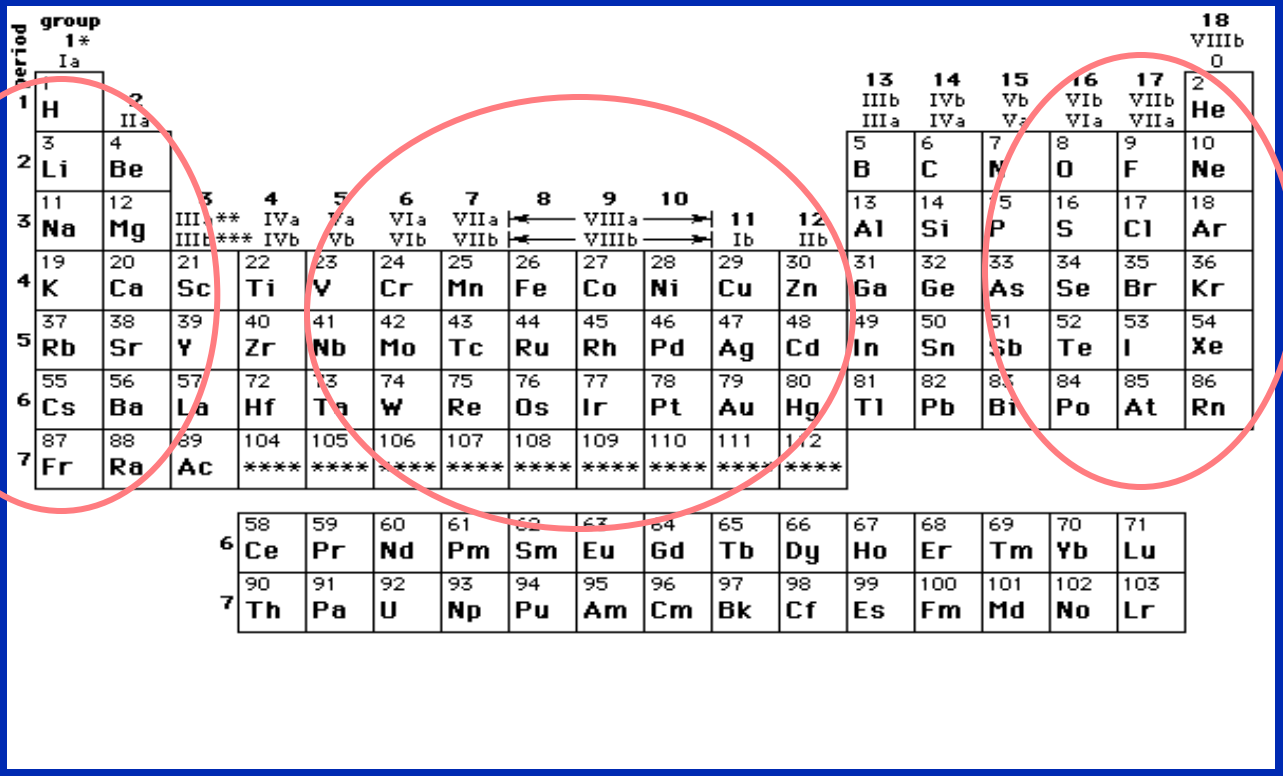
S.C.: n.n. at (±a, 0, 0); (0, ±a, 0); (0, 0, ±a)

$$\varepsilon(k) = -\alpha - 2\gamma\,[\,\cos(k_x a) + \cos(k_y a) + \cos(k_z a)\,]$$

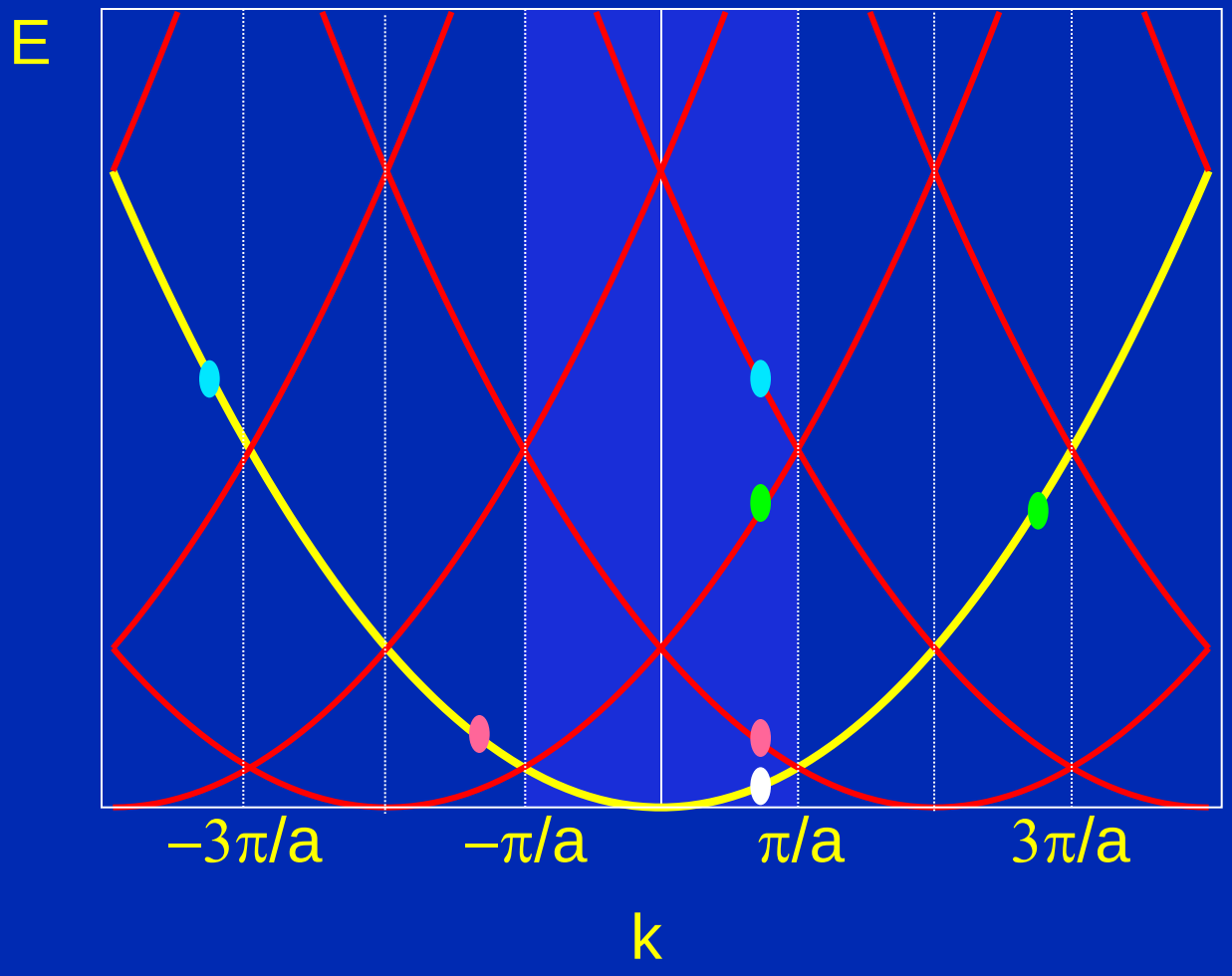


Tight binding

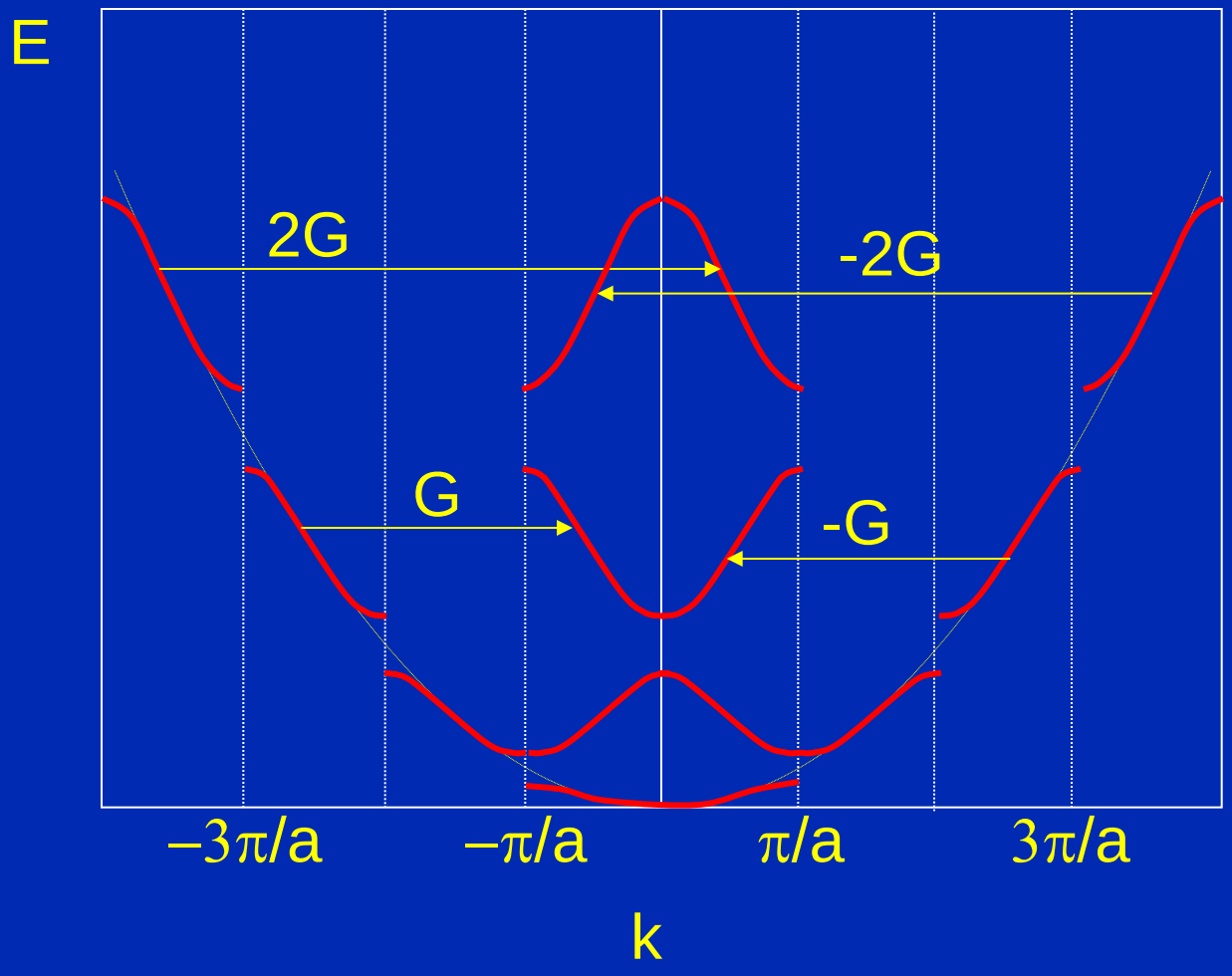
- TB method: Insulators and core electrons and d-electrons in transition metals (e.g. Cu, V, Ti etc.).
- Nearly free electron model: conduction electrons, s or p, alkali (e.g. Na, K, etc.)



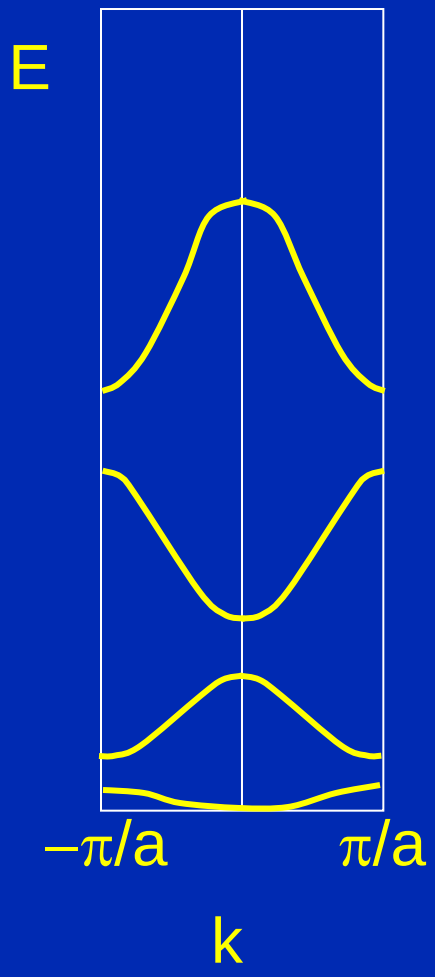
Reduced Brillouin zone



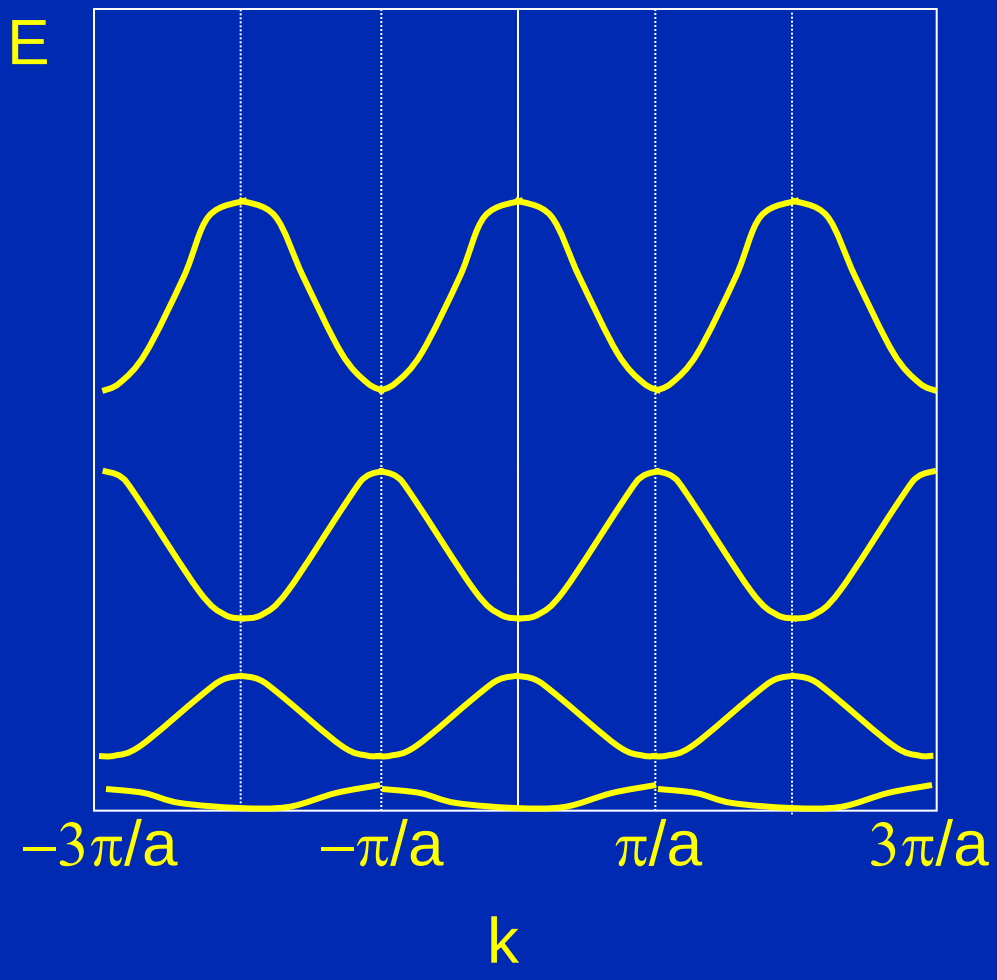
Extended zone scheme



Reduced zone scheme



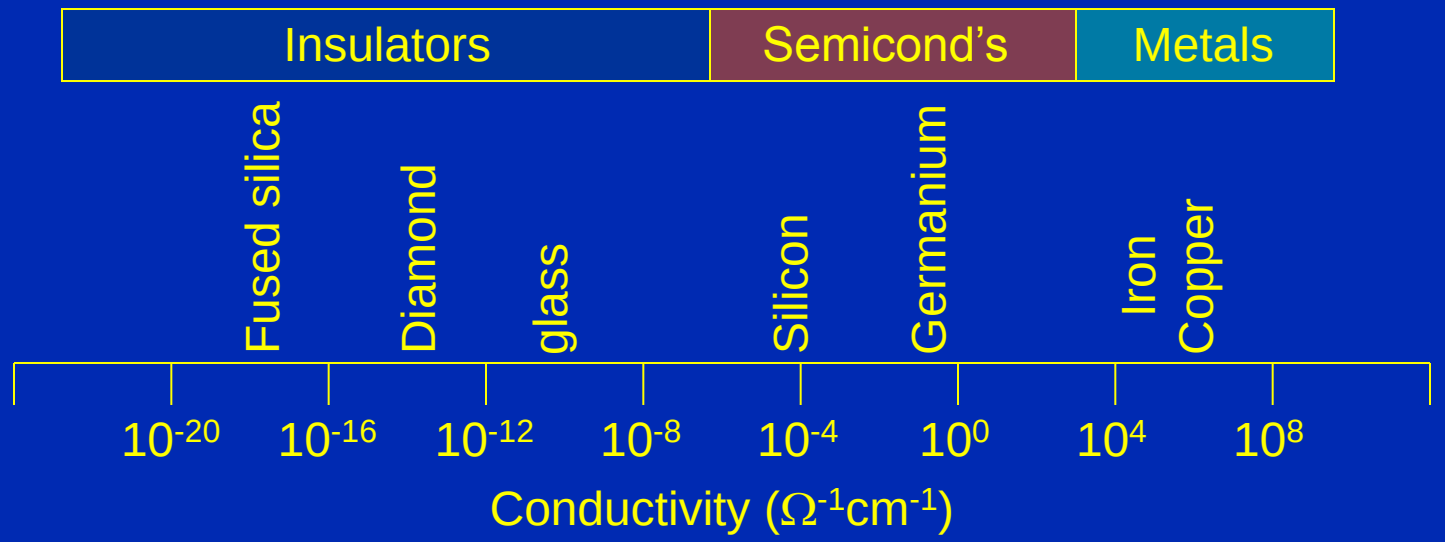
Periodic zone scheme



$$E_{n,\vec{k}+\vec{G}} \equiv E_{n,\vec{k}}$$

Bandstructure

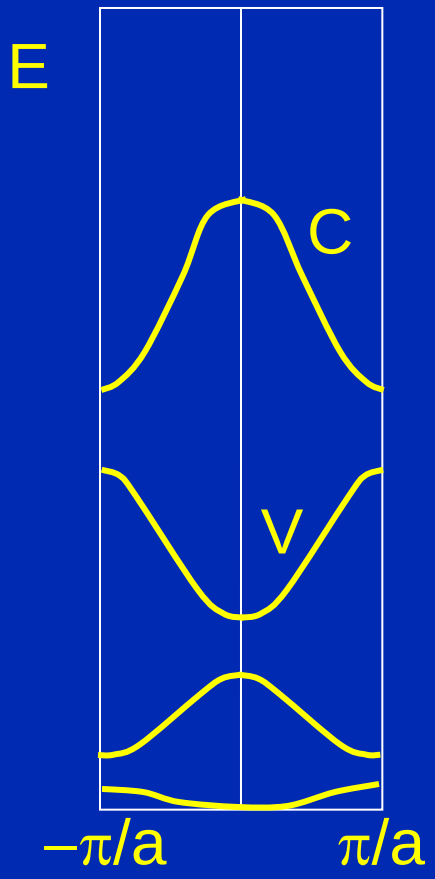
- Why are not all solids metals

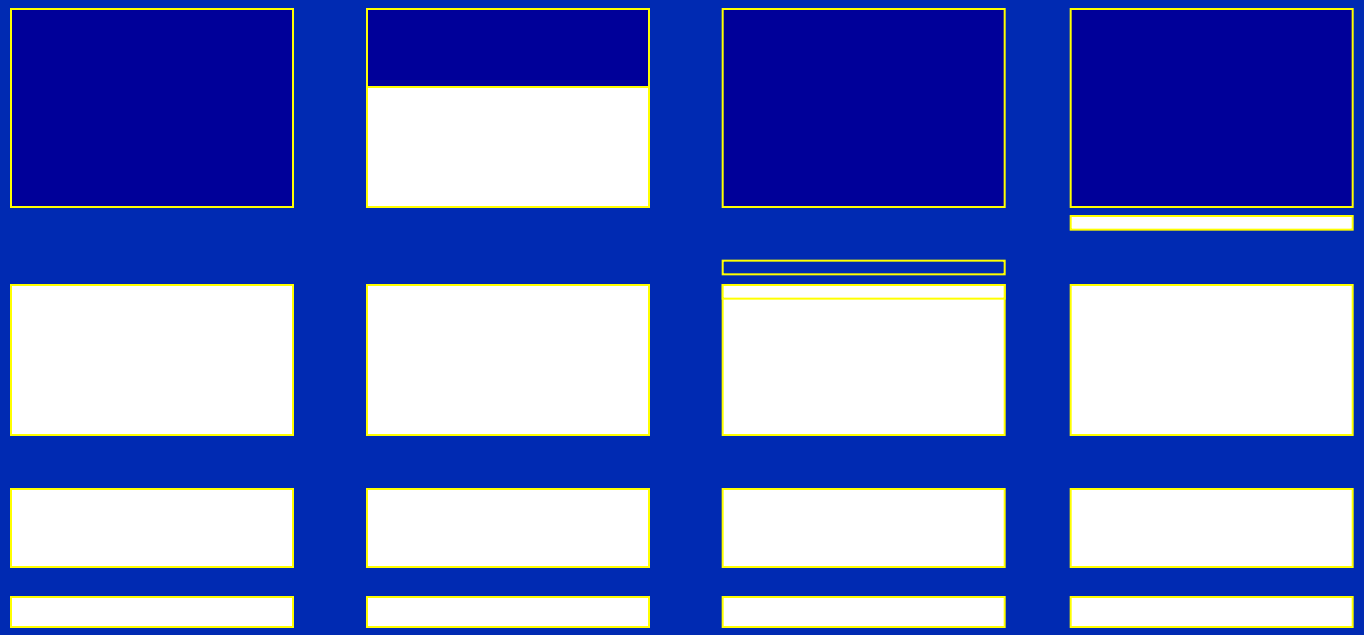


- Why is diamond an insulator
- Why is copper a metal
- Why does the conductivity of Si increase upon heating

Conductivity

$$\sigma = n \cdot e \cdot \mu$$





Insulator | Metal | p-Doped Semi-Conductor | n-Doped Semi-Conductor

Diamond and Germanium

Diamond (E_g=5.5 eV)

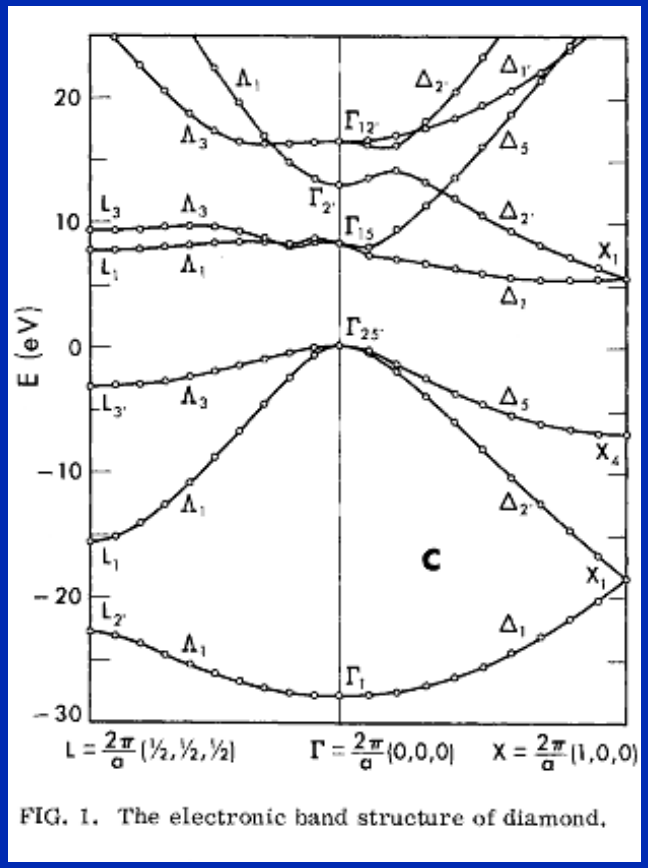
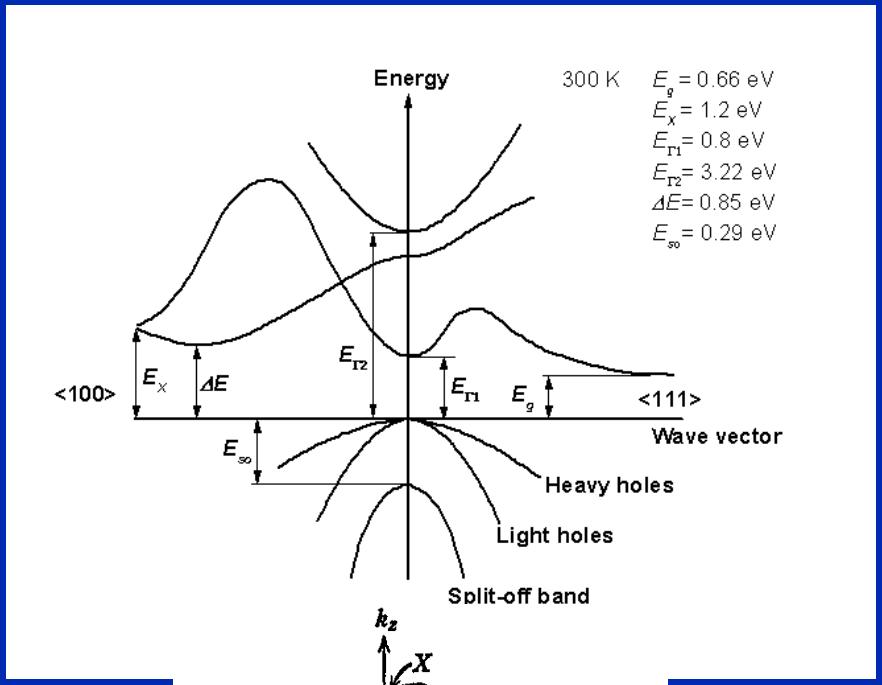
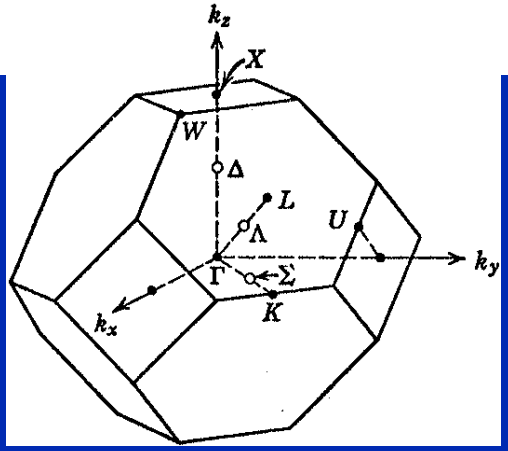


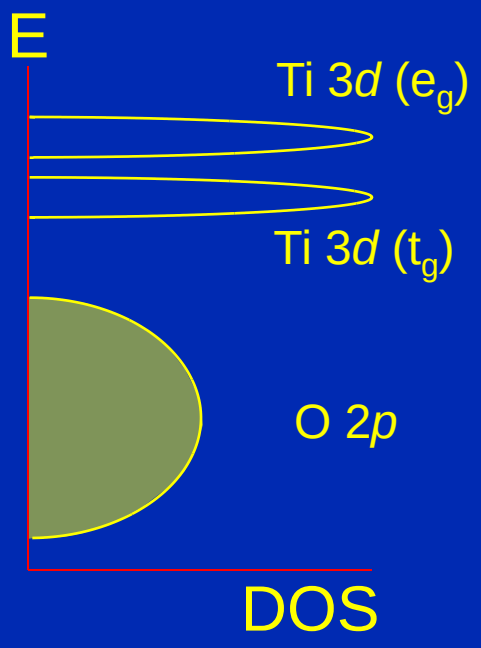
FIG. 1. The electronic band structure of diamond.

Germanium (E_g=0.7 eV)

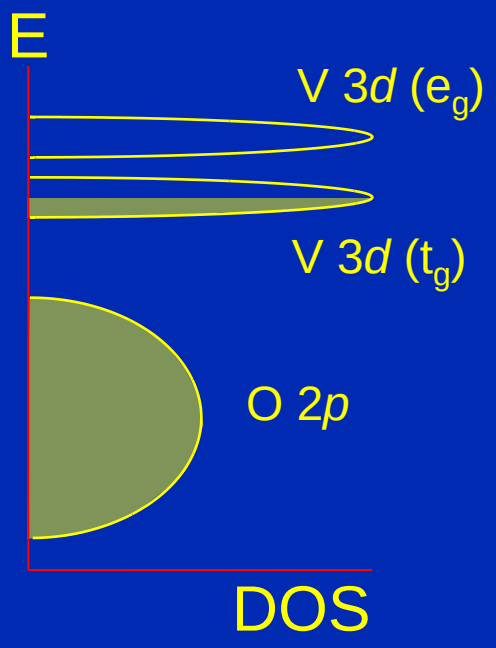




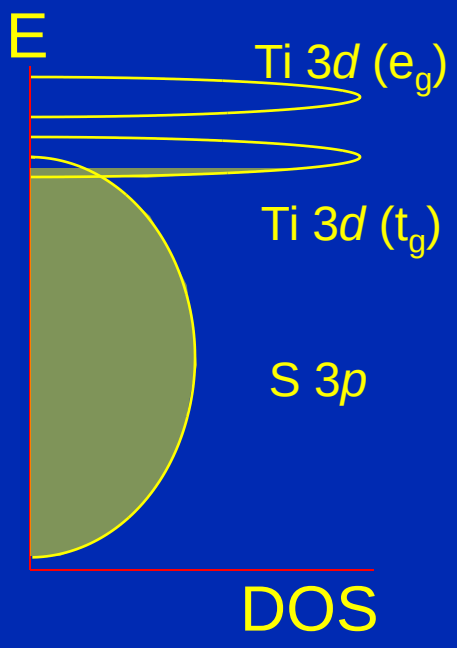
Bandfilling & overlap



TiO_2
Empty *d*-bands



VO_2
Partially filled *d*-bands

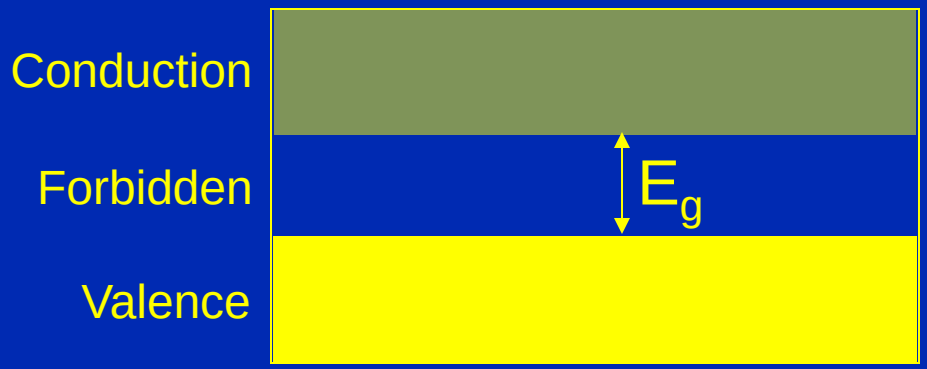


TiS_2
Overlapping bands

Ti: [Ar]$3d^2 4s^2$
V: [Ar]$3d^3 4s^2$

Band gap in some materials

		E_g(eV)
Diamond	I	5.4
Si	I	1.17
Ge	I	0.74
GaAs	d	1.52
GaSb	d	0.81
Te	d	0.33
ZnO		3.44
Cu_2O	d	2.17
CdTe	d	1.6
TiO_2		3.03



Direct & indirect
Optical absorption