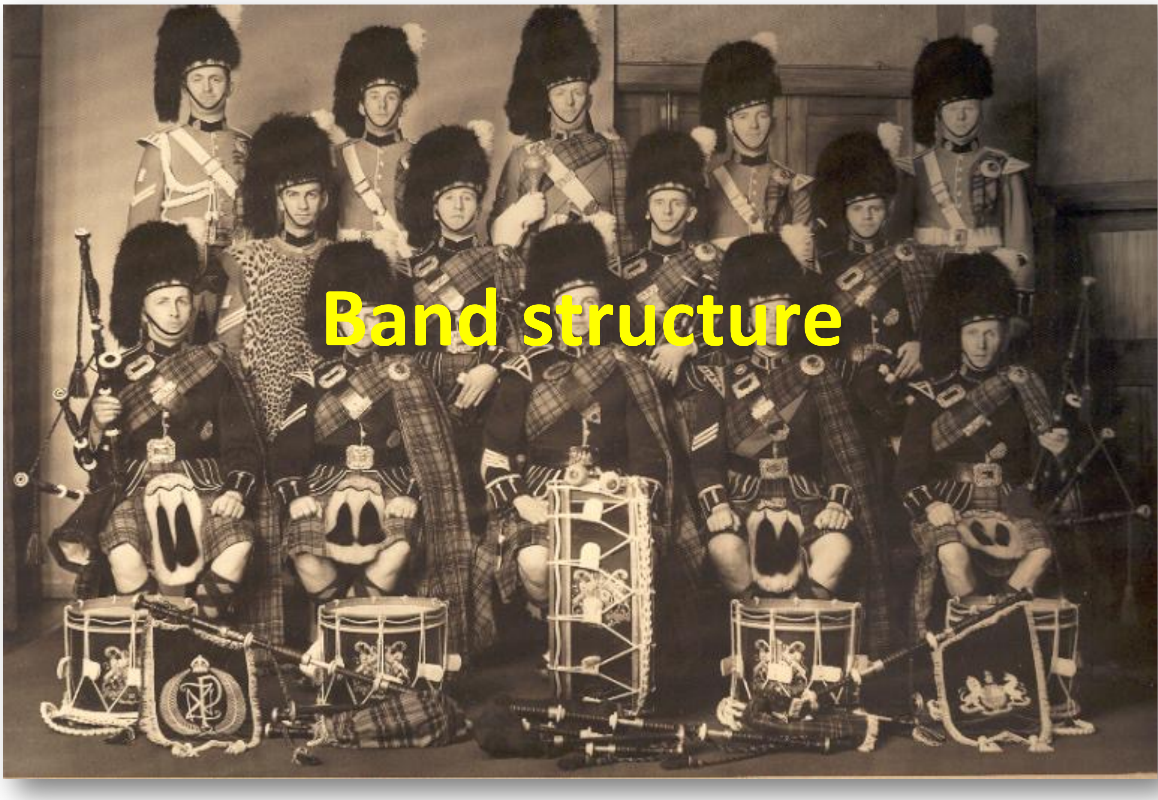
MSE 423 Fall 2025 – Week 10



$\vec{b}_1 = \frac{2\pi}{V} (\vec{a}_2 \times \vec{a}_3)$

Last week

$\vec{a}_1$

$\vec{a}_i \cdot \vec{b}_j = 2\pi \delta_{ij}$

- Direct Bravais lattices (14, in 7 classes (up to 4 types for each)
- Primitive, conventional, and Wigner-Seitz cell
- Reciprocal lattice, and Brillouin zones
- Hamiltonian in a periodic potential, and graphical representation
- Bloch theorem, in two forms
- From k in extended space to 1st BZ + band index

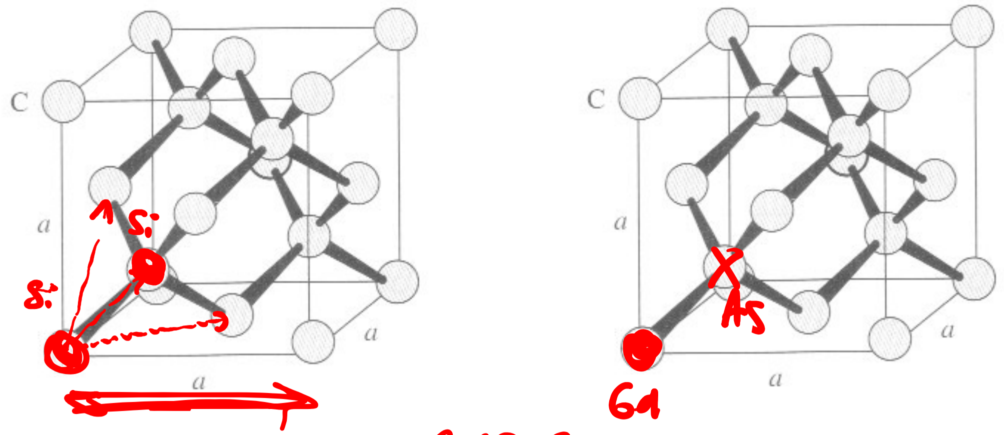
$e^{i(\vec{G}\cdot\vec{r})}$

$[\hat{H}, \hat{T}_{\vec{R}}] = 0 \Rightarrow \psi_{\vec{k}}(\vec{r}+\vec{R}) = e^{i\vec{k}\cdot\vec{R}} \psi_{\vec{k}}(\vec{r})$

$\Downarrow$

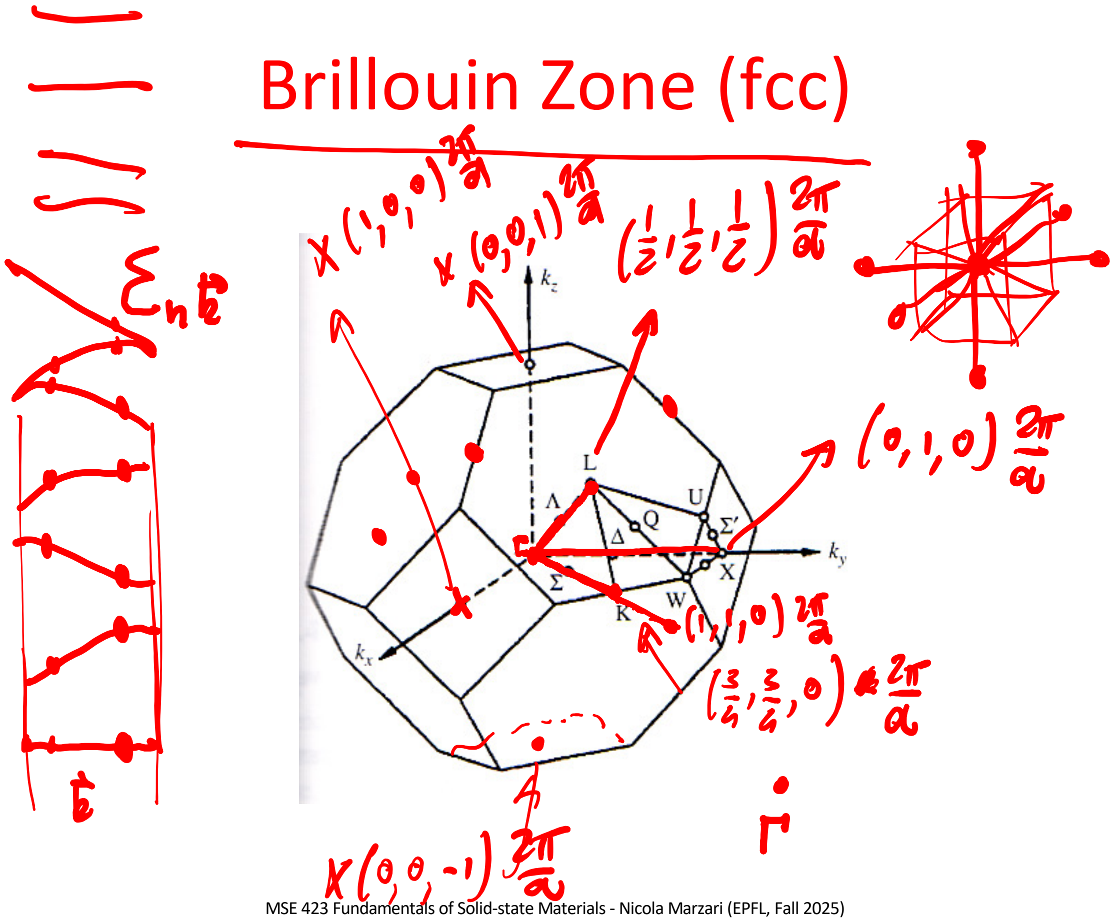
$\psi_{\vec{k}}(\vec{r}) = u_{\vec{k}}(\vec{r}) e^{i\vec{k}\cdot\vec{r}}$

Diamond and Zincblend

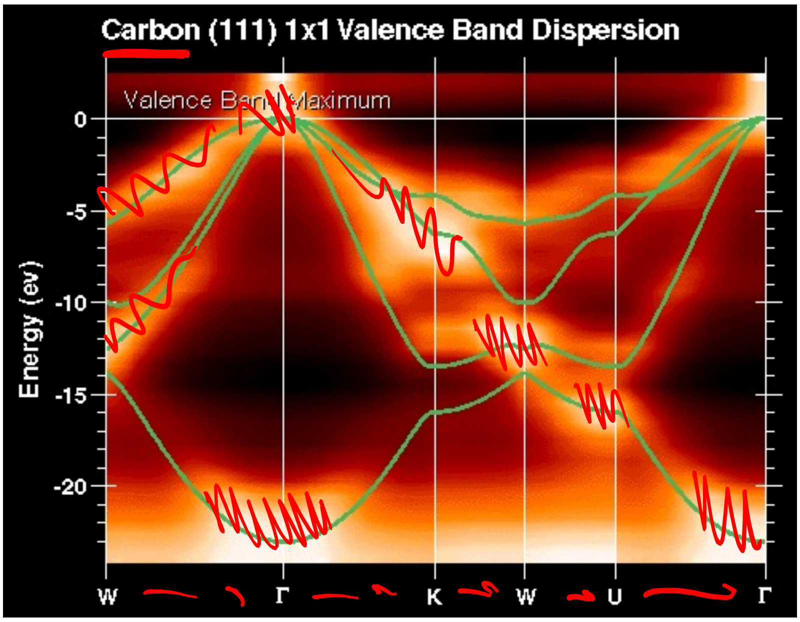


FCC + 2-ATOM BASIS

Brillouin Zone (fcc)

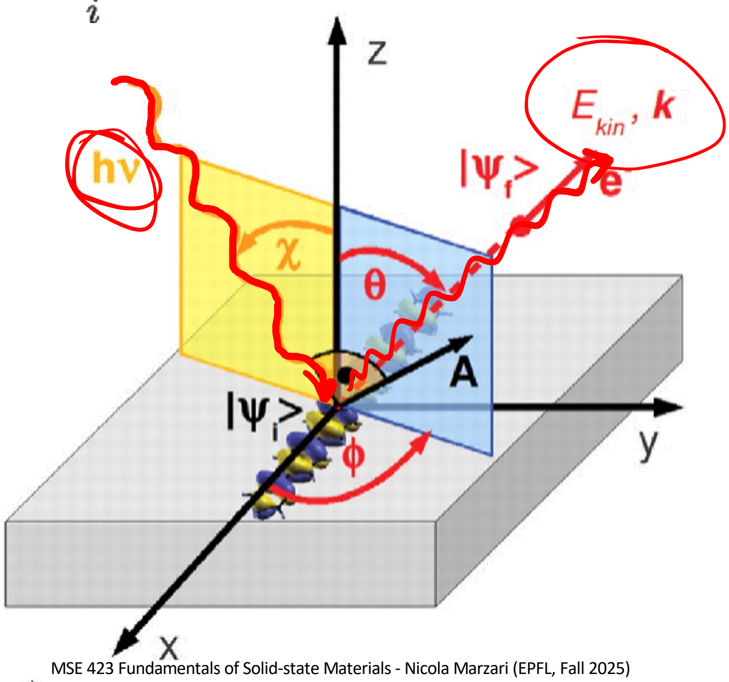


Band Structure of Diamond

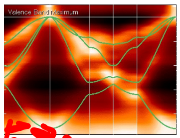


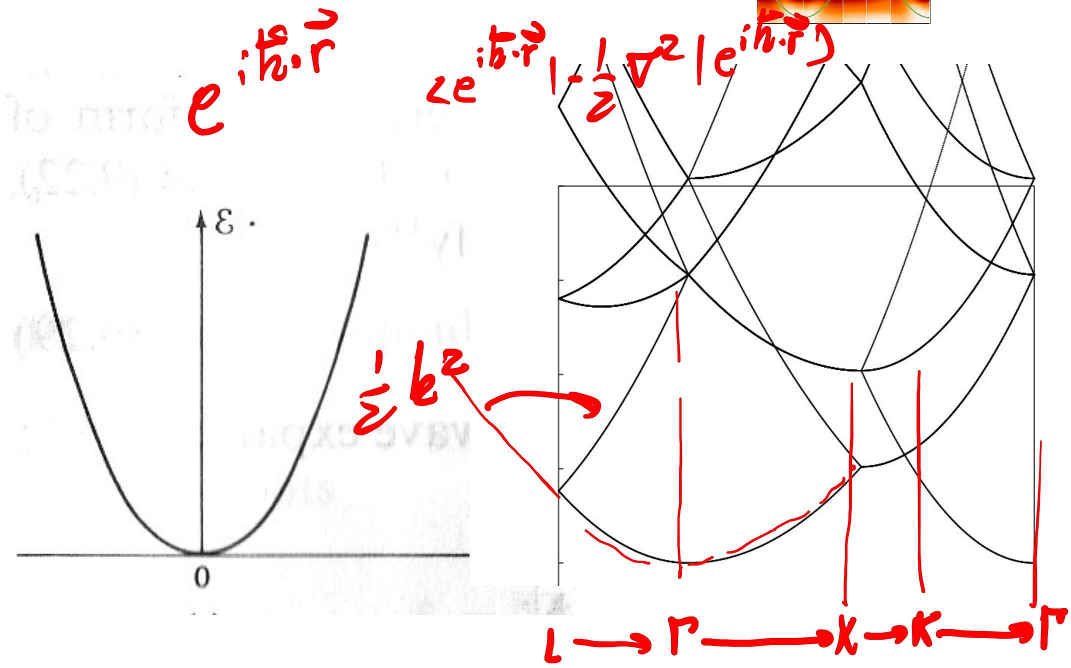
ARPES: Angle resolved photoemission spectroscopy

$$I(\omega) = \sum_i |\langle \varphi_f | \hat{H}_{\text{int}} | \varphi_i \rangle|^2 \delta(\epsilon_f - \epsilon_i - \hbar\omega)$$



Why does it look like this?





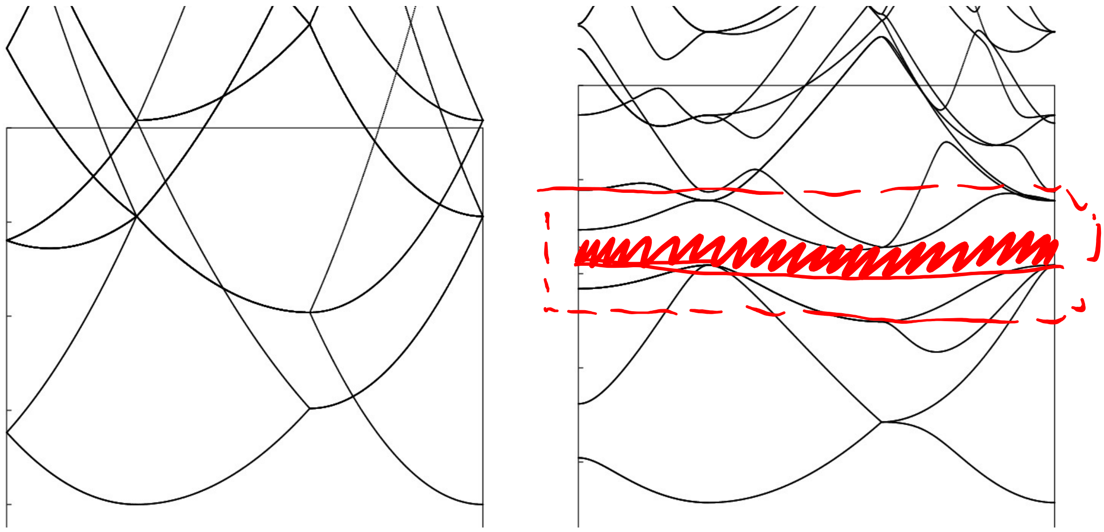
OSSCAR.ORG

https://osscar-quantum-mechanics.materialscloud.io/voila/render/index.ipynb

Section 2: **Band Theory of Crystals**

1. Fourier Transforms and Plane-Wave Expansions
2. Brillouin Zone
3. Free-Electron Bandstructure
4. Density of States
5. Norm-conserving Pseudopotentials

Band Structures: Free Electron Gas, Silicon

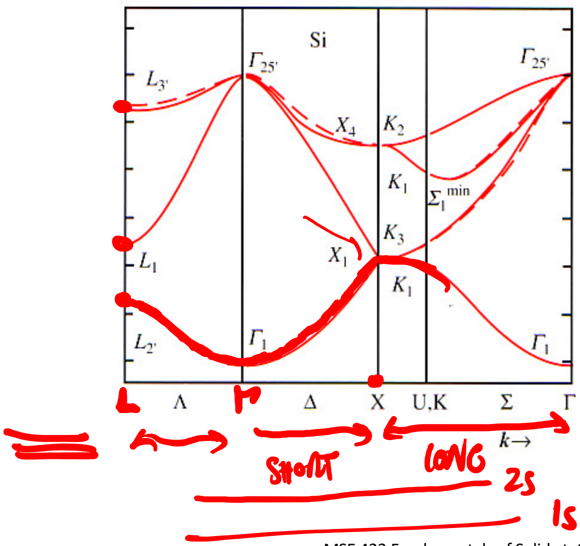


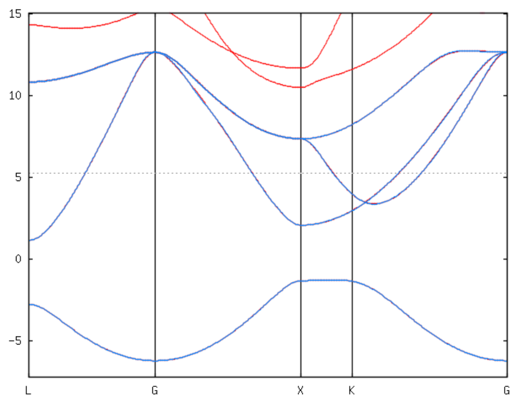
Silicon ~~Lead~~

$-\frac{1}{4}\psi$

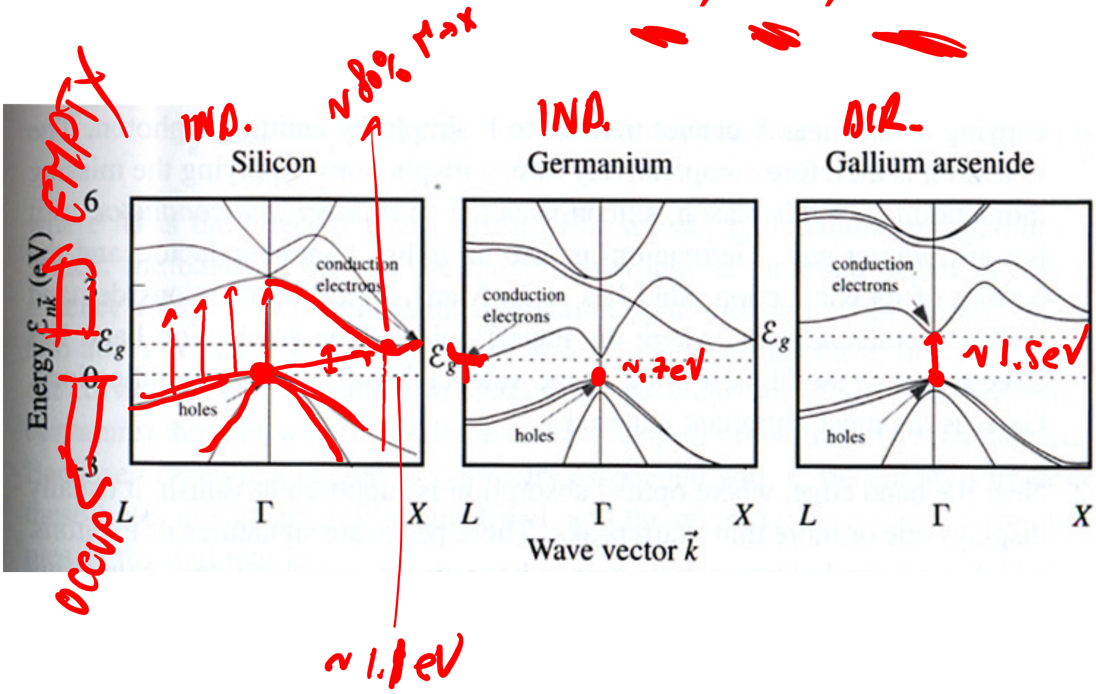
$-\frac{1}{4}\psi$

-1ψ





Band structure of Si, Ge, GaAs



Conduction band minima (in 3d)

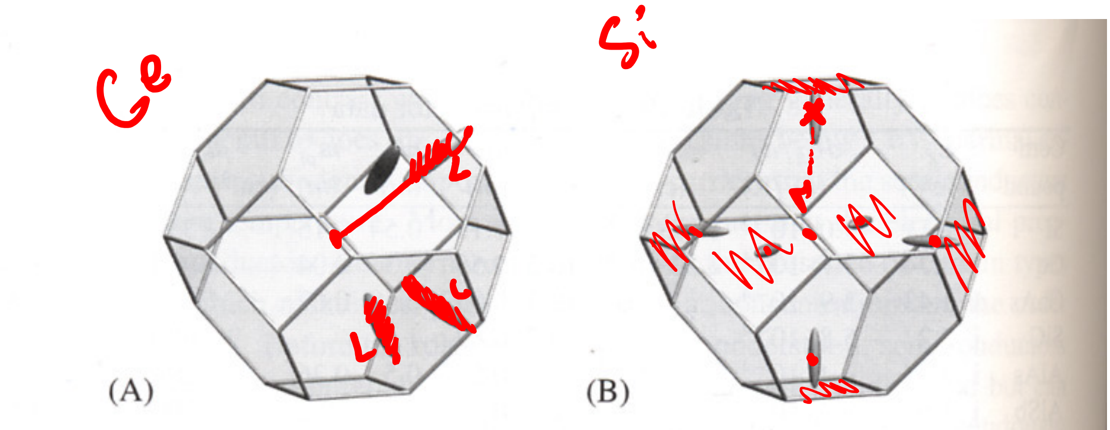


Figure 19.9. (A) The conduction band minima in germanium lie along (111) and straddle the zone boundary, producing four inequivalent pockets of electrons with a highly anisotropic effective mass. (B) In silicon, the conduction band minima lie 8/10 of the way toward (100), producing six pockets of electrons, but only three with distinct symmetries.

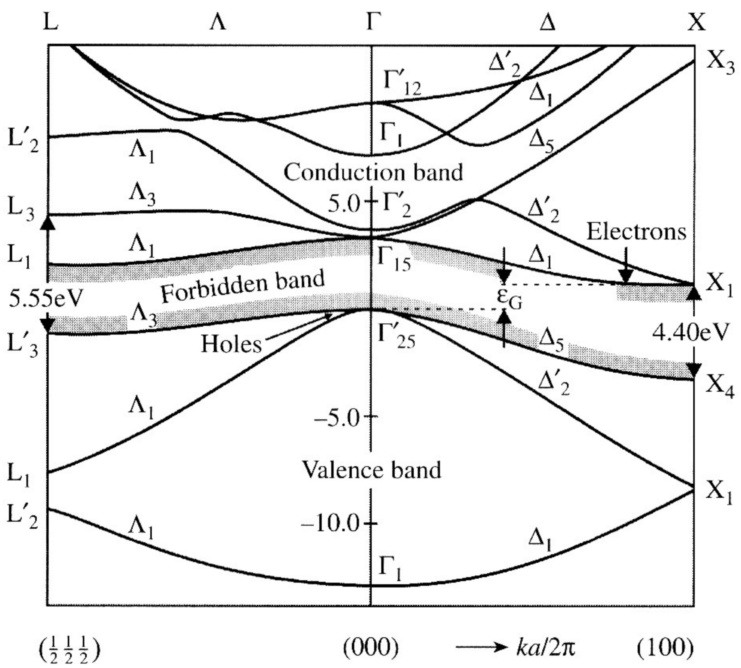
Impress your examiners (orals)

Table 19.1. Semiconductor data

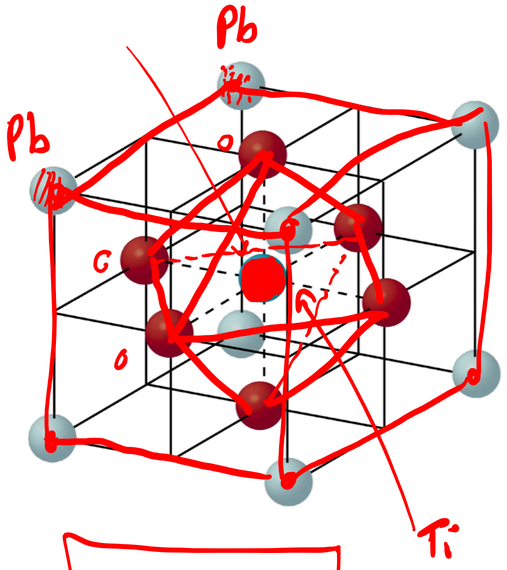
Compound		$\mathcal{E}_g$ (eV)	$d\mathcal{E}_g/dT$ (eV/K)	n_i (cm^{-3})	ϵ^0	$m_n^\star$ (m)	$m_{ph}^\star$ (m)	$m_{pl}^\star$ (m)	μ_n (cm^2/V s)	μ_p (cm^2/V s)
Si	i	1.11	$-9.0\cdot10^{-5}$	$1.02\cdot10^{10}$	11.9	1.18	0.54	0.15	1350	480
Ge	i	0.74	$-3.7\cdot10^{-4}$	$2.33\cdot10^{13}$	16.5	0.55	0.3	0.04	3900	1800
GaAs	d	1.43	$-3.9\cdot10^{-4}$	$2\cdot10^{6}$	12.5	0.067	0.50	0.07	7900	450
SiC	i	2.2	$-5.8\cdot10^{-4}$		9.7	0.82	1		900	50
AlAs	i	2.14	$-4\cdot10^{-4}$	$2\cdot10^{17}$	10.0	0.5	0.5	0.26	294	
AlSb	i	1.63	$-4\cdot10^{-4}$		12.0	0.3	1	0.5	200	400
GaN	d	3.44	$-6.7\cdot10^{-4}$	$2\cdot10^{17}$	12.0	0.3	1		440	
GaSb	d	0.7	$-3.7\cdot10^{-4}$	10^{14}	15.7	0.05	0.3	0.04	7700	1600
InP	d	1.34	$-2.9\cdot10^{-4}$	$1.2\cdot10^{8}$	15.2	0.073	0.6	0.12	5400	150
InAs	d	0.36	$-3.5\cdot10^{-4}$	$1.3\cdot10^{15}$	15.2	0.027	0.4	0.03	30 000	450
InSb	d	0.18	$-2.8\cdot10^{-4}$	$2.0\cdot10^{16}$	16.8	0.013	0.4	0.02	77 000	850

Data on whether a compound has a direct (d) or indirect (i) gap, energy gap, static dielectric constant, effective masses, and mobilities, for some semiconductors. The electron effective mass $m_n^\star$ is the density of states effective mass defined in Eq. (19.23). The data refer to room temperature, and to samples with donor and acceptor impurities at densities of 10^{15} cm^{-3} or less. Source: Landolt and Börnstein (New Series) vol. 17 and Pierret (1996).

Valence+conduction bands in Si



Perovskites



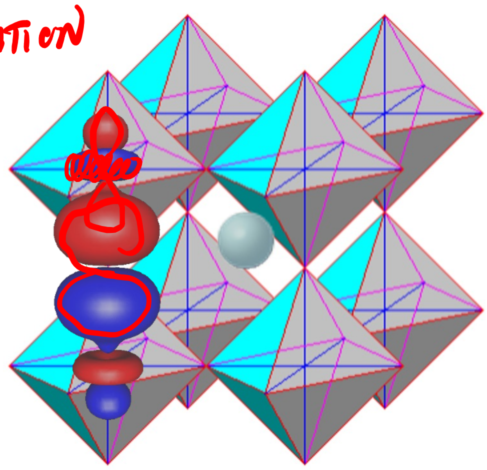
A CATIONS

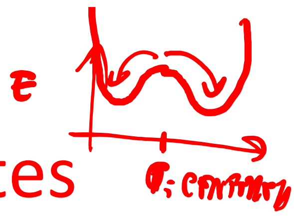
OXYGEN (N, S)

B CATION

$\boxed{ABO_3}$

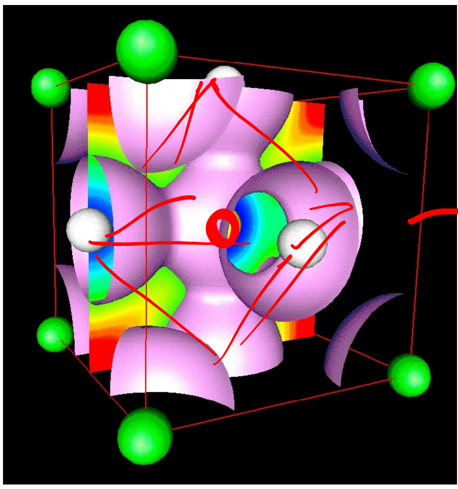
$\boxed{PbTiO_3}$



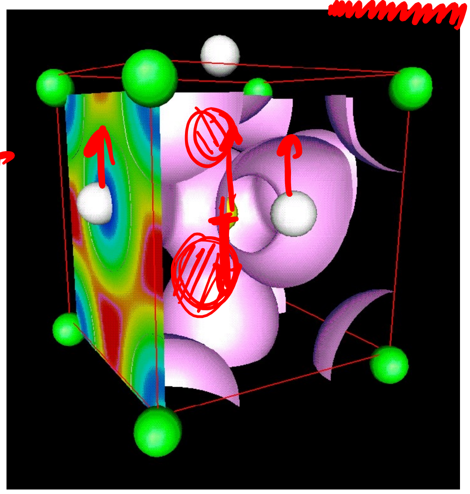


Ferroelectric perovskites

CUBIC $PbTiO_3$ | TETRAGONAL $PbTiO_3$



LOW T



$Pb^{2+}|Ti^{4+}|O_3^{-2}$ $PbTiO_3$

Ferroelectric perovskites

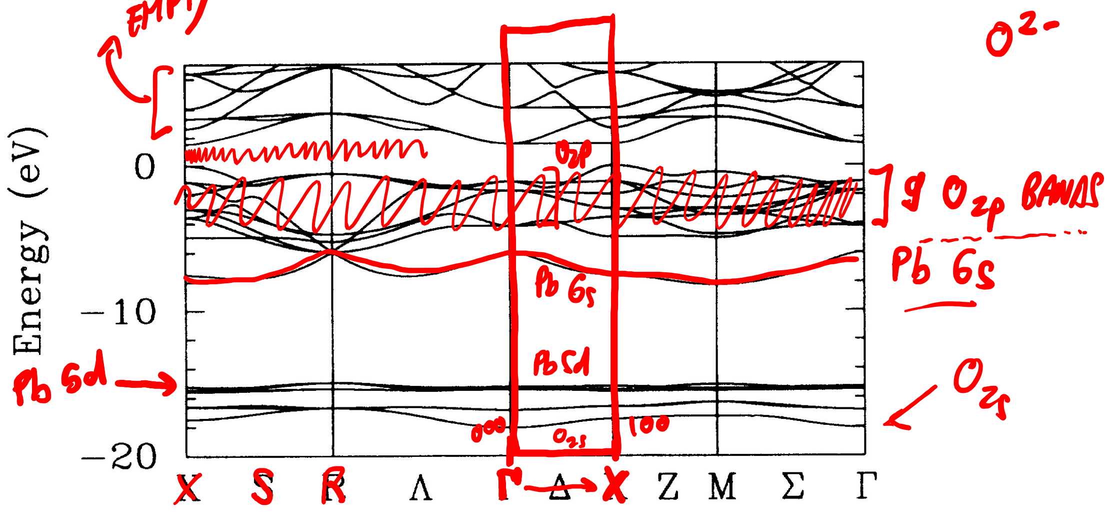
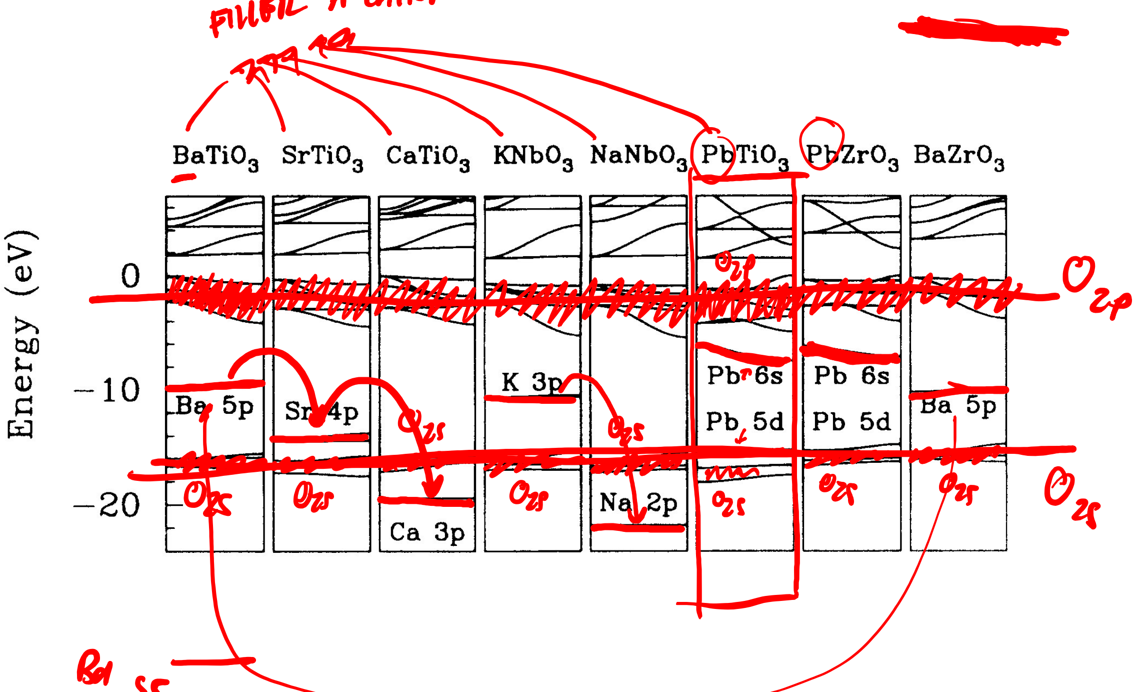


FIG. 3. Band structure of cubic $PbTiO_3$ for selected high-symmetry directions.

ABO_3 → 3 OXYGENS

Ferroelectric perovskites

FILLER A CATION



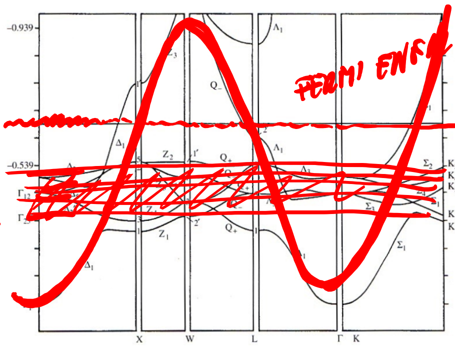
FCC METALS
1 AT/UNIT CELL

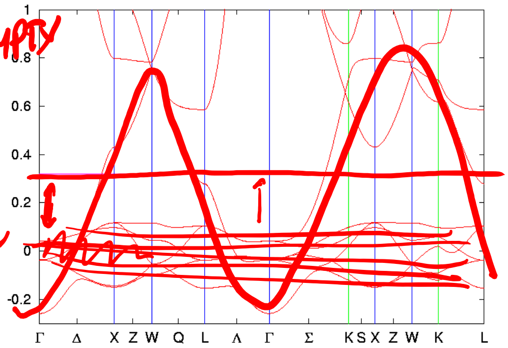
Copper

Silver

$3d^{10}4s^{1}$

FERMI ENERGY
EMPTY
10e
FULL





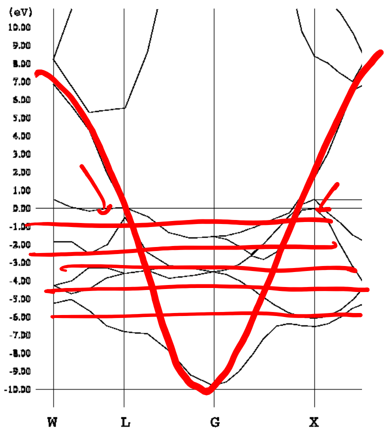
BERGSTRESSER & COHEN
PHYS. REV. 1966

Platinum

Gold

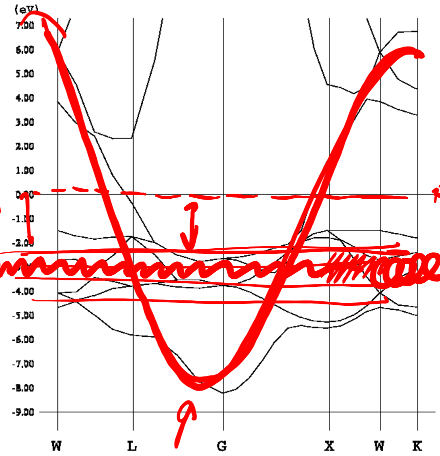
PtO

LARGEST



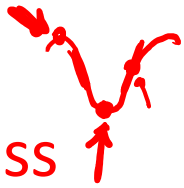
Pt(fcc) a=7.56a.u.

FERMI



Au(fcc) a=8.2a.u

Group velocity, effective mass



FREE ELECTRON $\varepsilon_k = \frac{\hbar^2 k^2}{2m}$

GROUP VELOCITY

$$\vec{v}_n = \frac{1}{\hbar} \vec{\nabla}_{\vec{k}} \varepsilon_n(\vec{k})$$

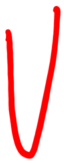
$$= \frac{1}{\hbar} \frac{\hbar^2}{2m} 2\vec{k} = \frac{\hbar}{m} \vec{k} = \frac{\vec{p}}{m} = \vec{v}$$

EFFECTIVE MASS

$$m_n^* = \hbar^2 \left(\frac{\partial^2 \varepsilon_n(\vec{k})}{\partial k^2} \right)^{-1}$$

IF $\varepsilon(\vec{k})$ IS QUADRATIC

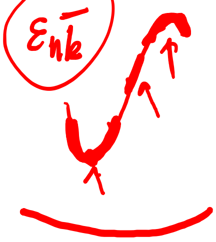
$$= \hbar^2 \left(\frac{\hbar^2}{2m} 2 \right)^{-1} =$$



$$= \hbar^2 m / \hbar^2 = m$$

LIGHT ELECTRON

$\varepsilon_{n\vec{k}}$



HEAVY ELECTRON