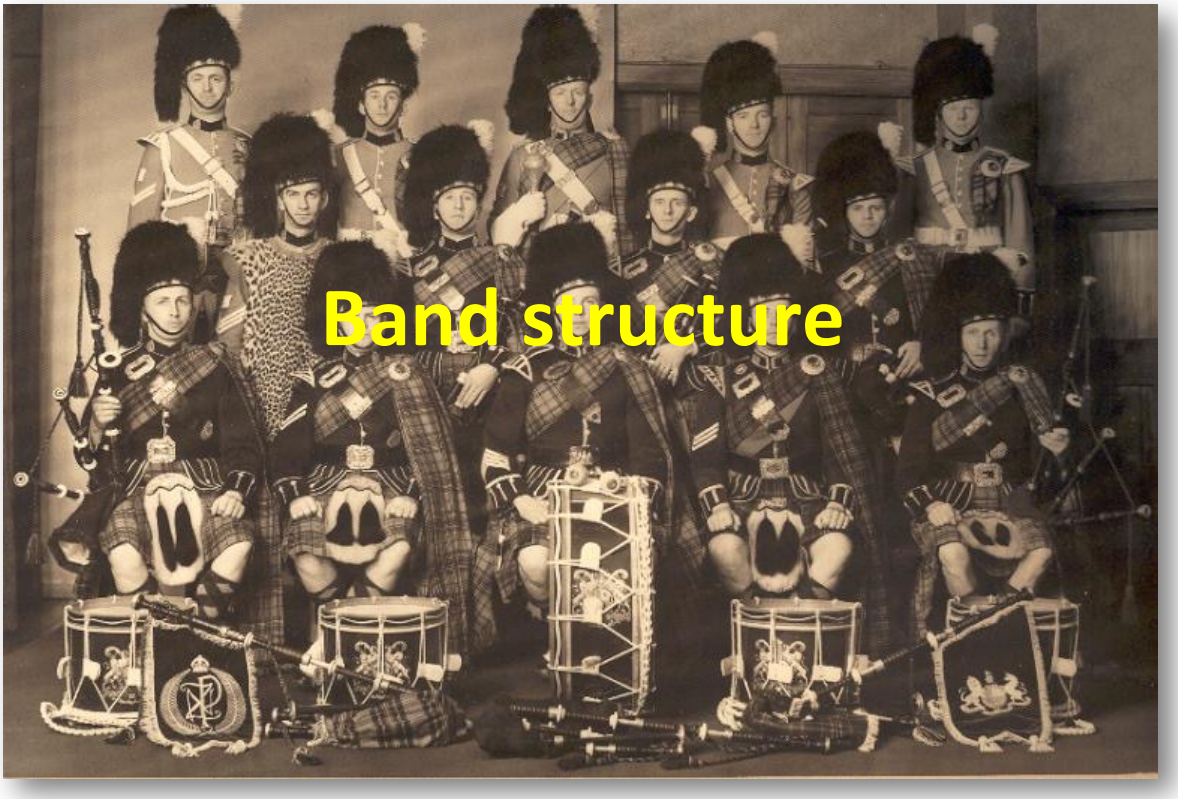
# MSE 423 Fall 2025 – Week 10

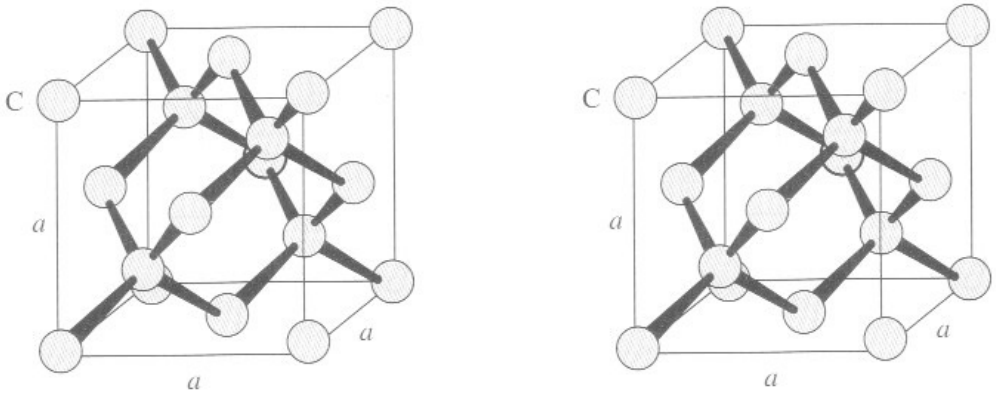





## Last week

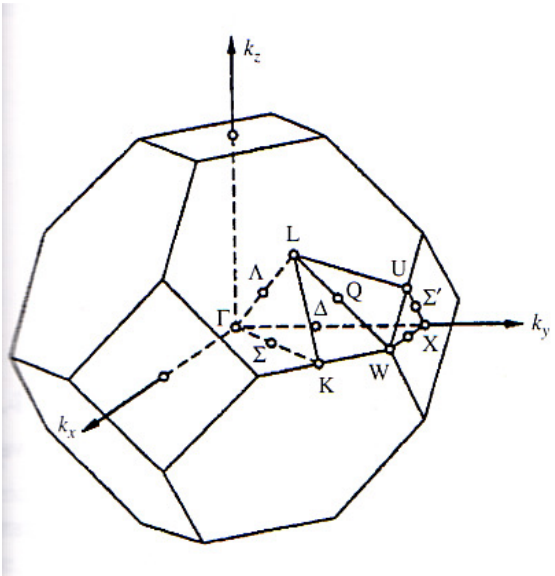
- Direct Bravais lattices (14, in 7 classes (up to 4 types for each)
- Primitive, conventional, and Wigner-Seitz cell
- Reciprocal lattice, and Brillouin zones
- Hamiltonian in a periodic potential, and graphical representation
- Bloch theorem, in two forms
- From k in extended space to 1$^{st}$ BZ +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

# Diamond and Zincblend

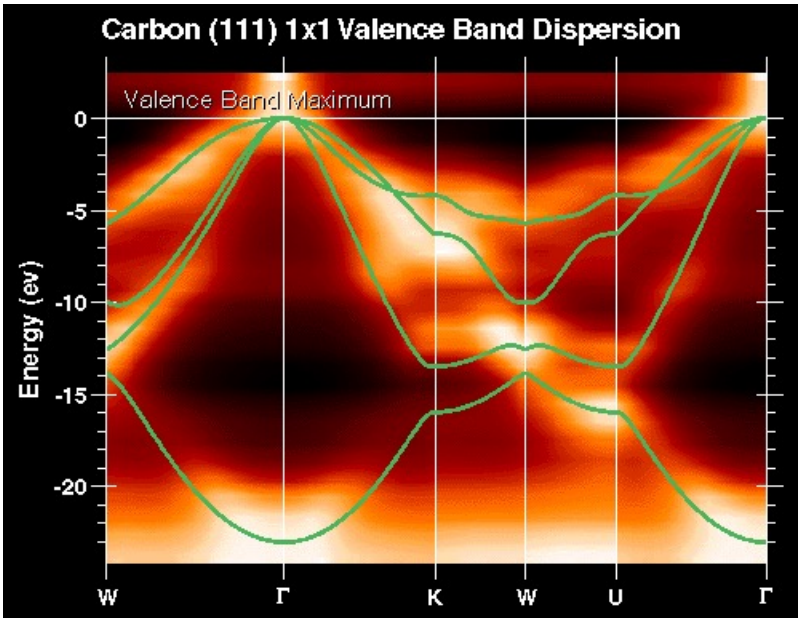





# Brillouin Zone (fcc)



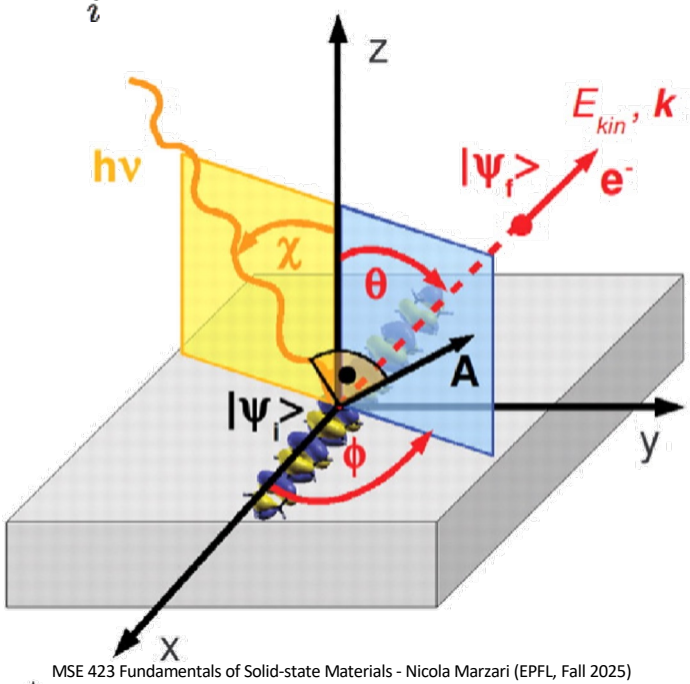
# Band Structure of Diamond



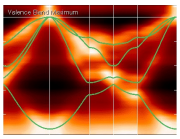


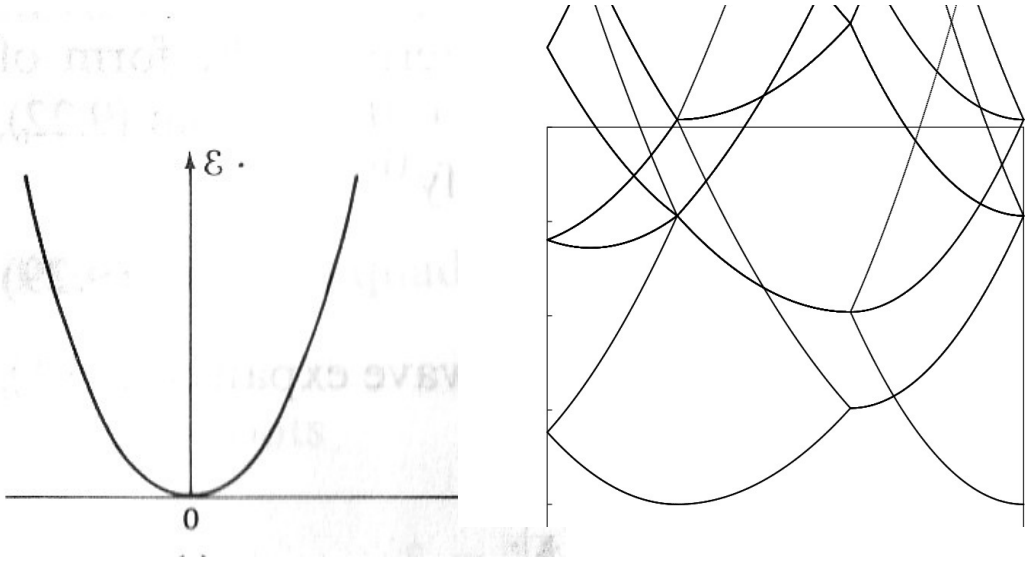

# ARPES: Angle resolved photoemission spectroscopy

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



# Why does it look like this?





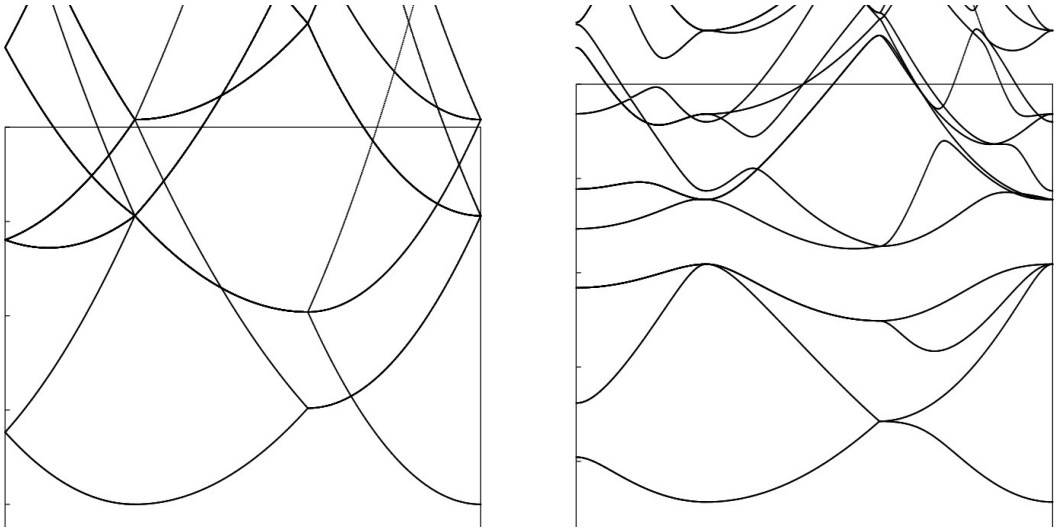



https://osscar-quantum-mechanics.materialscloud.io/voila/render/index.ipynb

## 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

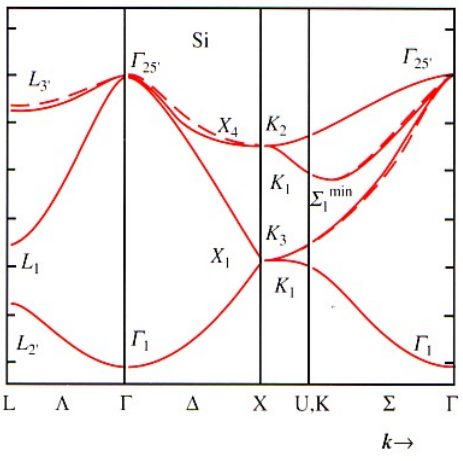
# Band Structures: Free Electron Gas, Silicon

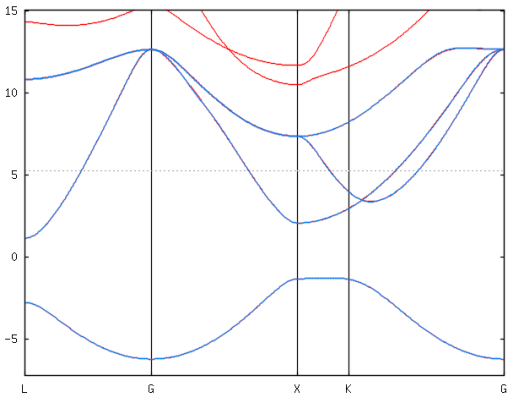




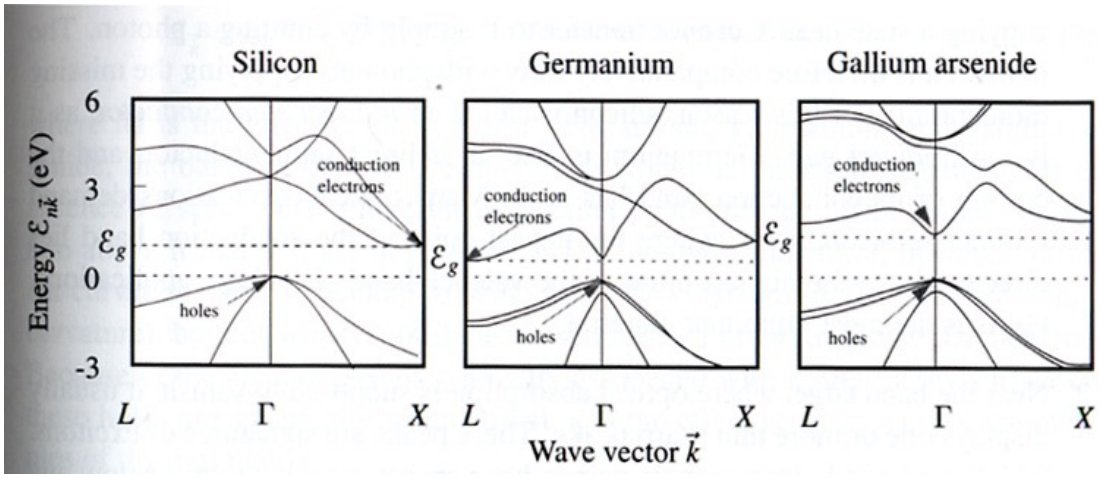
## Silicon

## Lead



# Band structure of Si, Ge, GaAs






# Conduction band minima (in 3d)

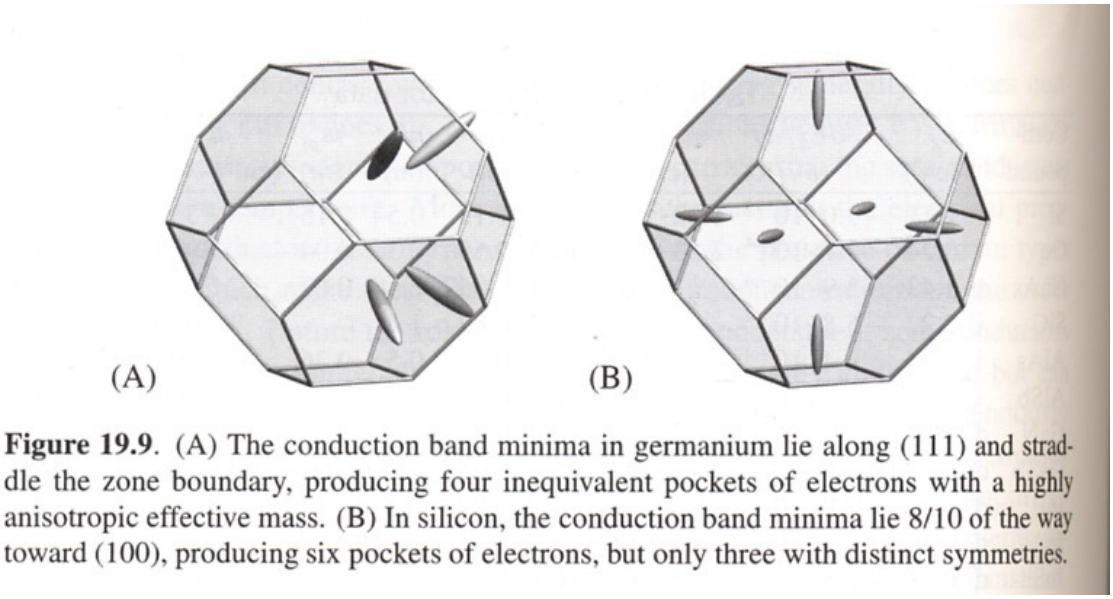



**Figure 19.9**. (A) The conduction band minima in germanium lie along (111) and straddle the zone boundary, producing four inequivalent pockets of electrons with a highly anisotropic effective mass. (B) In silicon, the conduction band minima lie 8/10 of the way toward (100), producing six pockets of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

# Impress your examiners (orals)

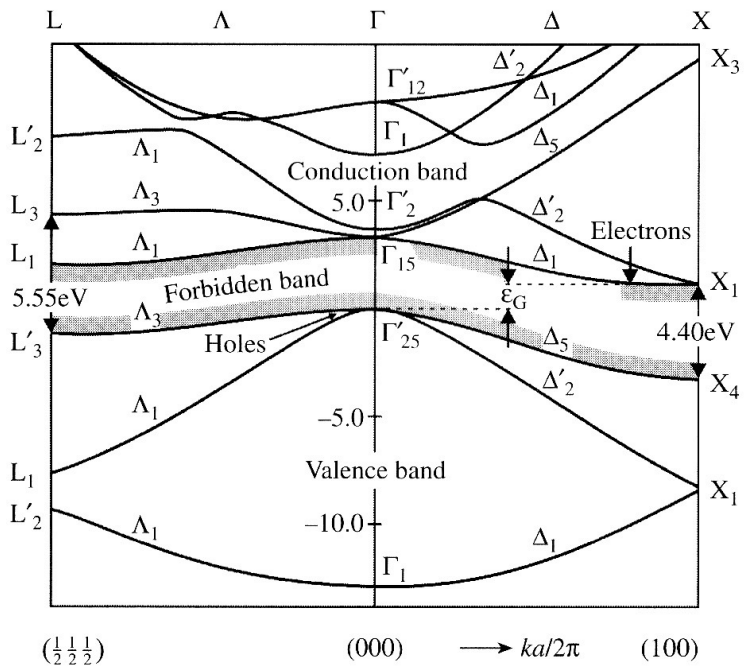
**Table 19.1.** Semiconductor data

| Compound | | $\mathcal{E}_g$ (eV) | $d\mathcal{E}_g/dT$ (eV/K) | $n_i$ ($cm^{-3}$) | $\epsilon^0$ | $m_n^\star$ ($m$) | $m_{ph}^\star$ ($m$) | $m_{pl}^\star$ ($m$) | $\mu_n$ ($cm^2/V\,s$) | $\mu_p$ ($cm^2/V\,s$) |
|---|---|---|---|---|---|---|---|---|---|---|
| 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 |

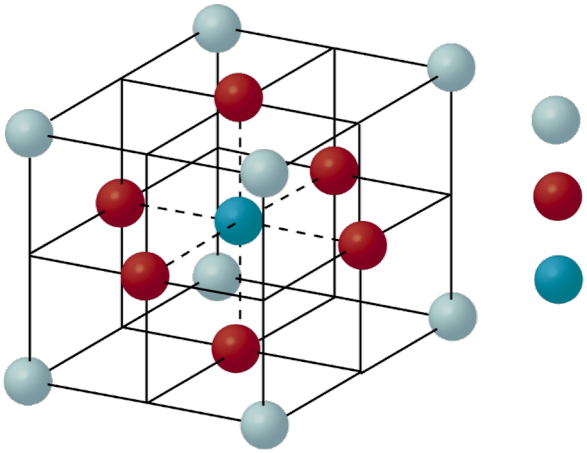
Data on whether a compound has a direct (d) or indirect (i) gap, energy gap, static dielectric constant, effective masses, and mobilities, for some semiconductors. The electron effective mass $m_n^\star$ is the density of states effective mass defined in Eq. (19.23). The data refer to room temperature, 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).

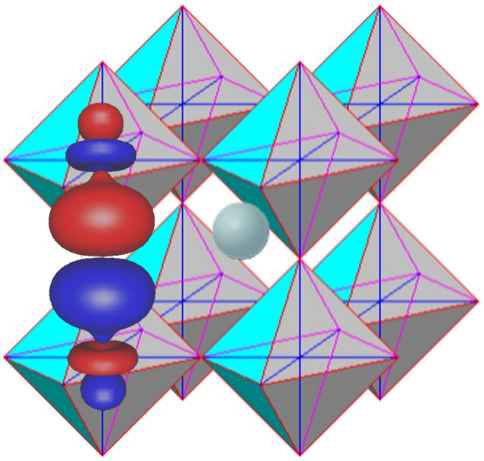


# Valence+conduction bands in Si



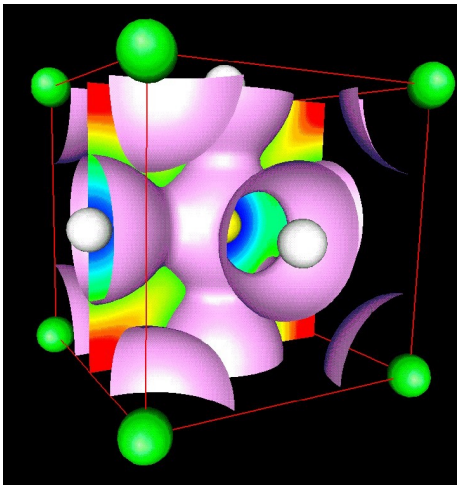
# Perovskites

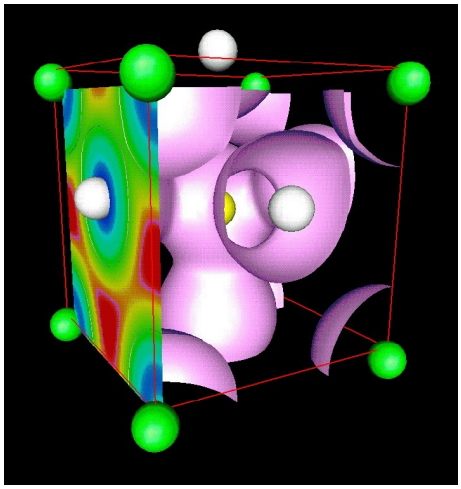






# Ferroelectric perovskites





# Ferroelectric perovskites

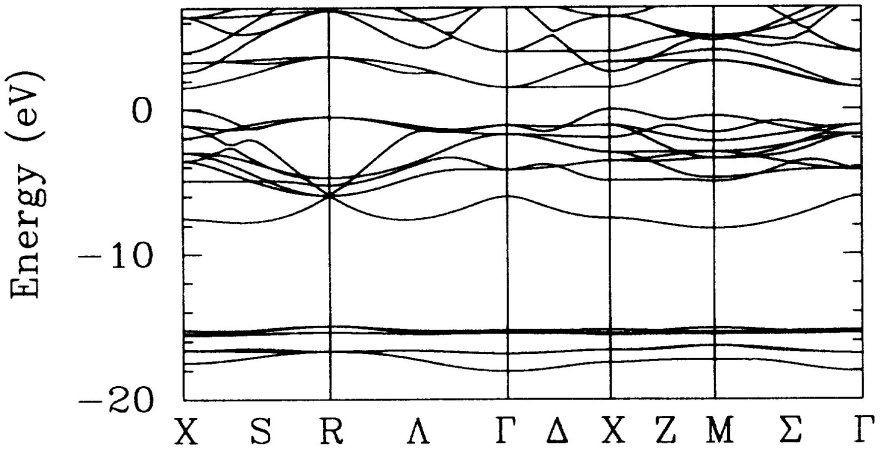
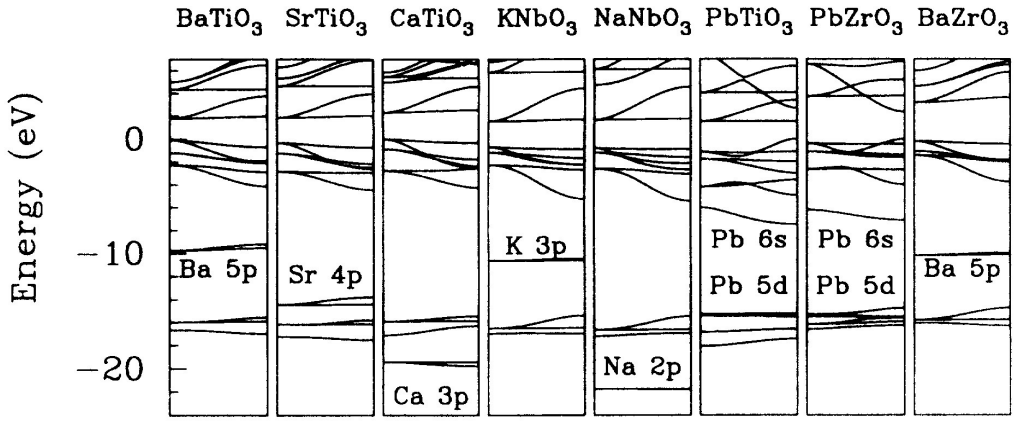


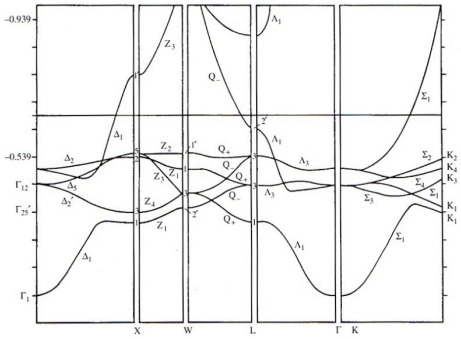

FIG. 3. Band structure of cubic $PbTiO_3$ for selected high-symmetry directions.



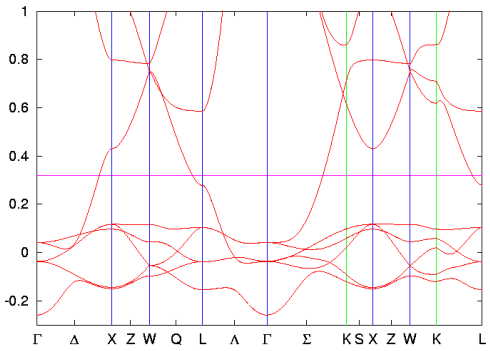
# Ferroelectric perovskites



# Copper

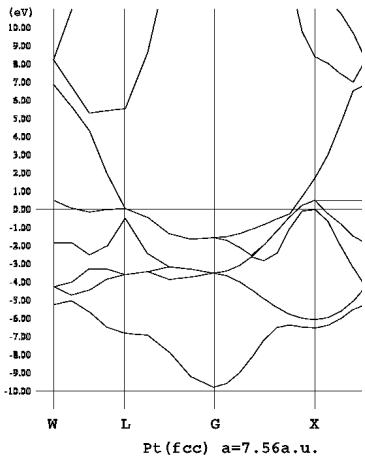



# Silver

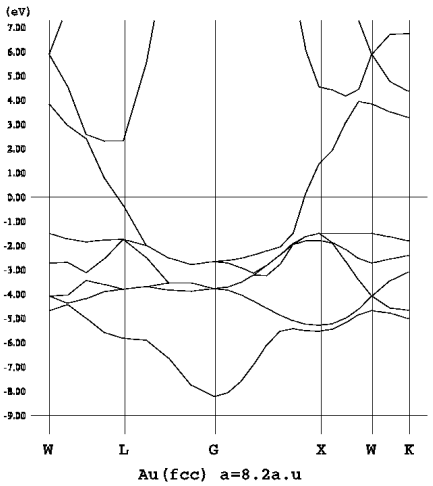





# Platinum



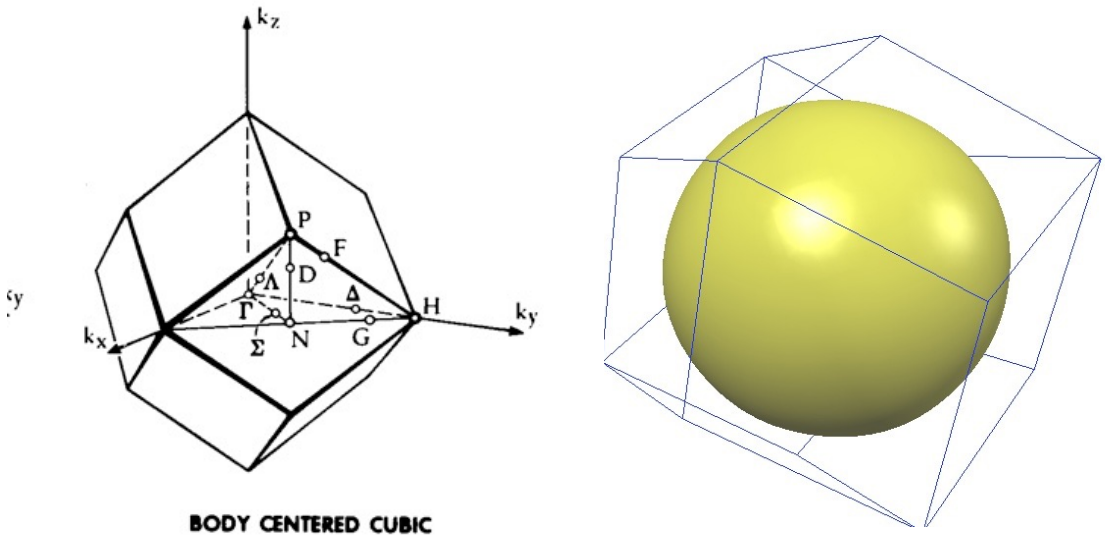

# Gold



# Group velocity, effective mass

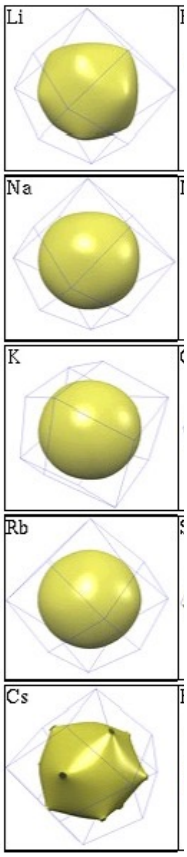


# The Fermi surface

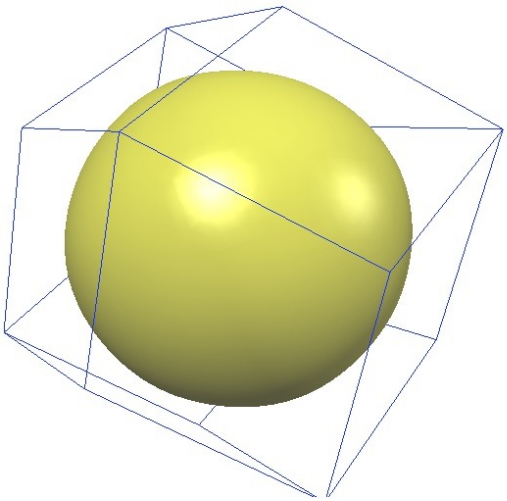



BODY CENTERED CUBIC

# The Fermi surface

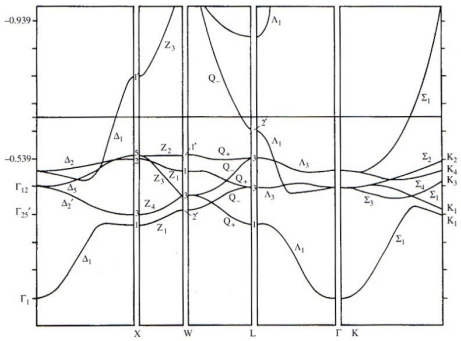


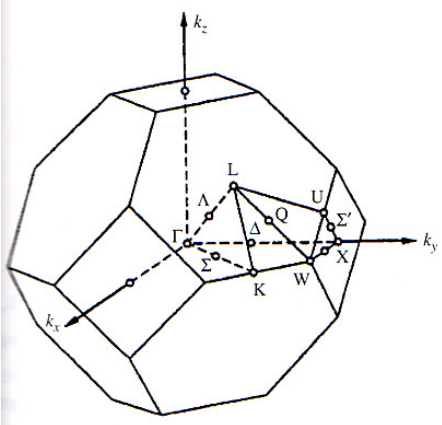

K



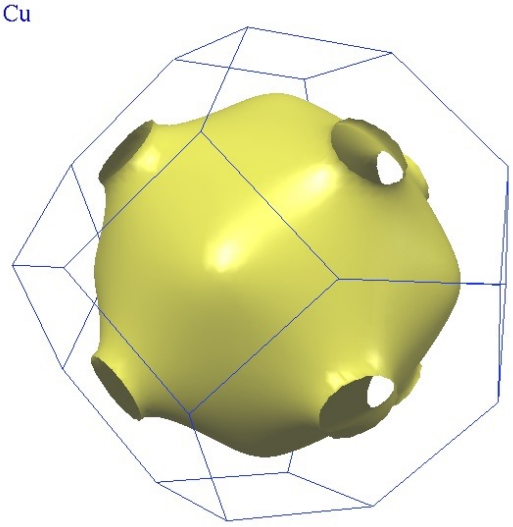


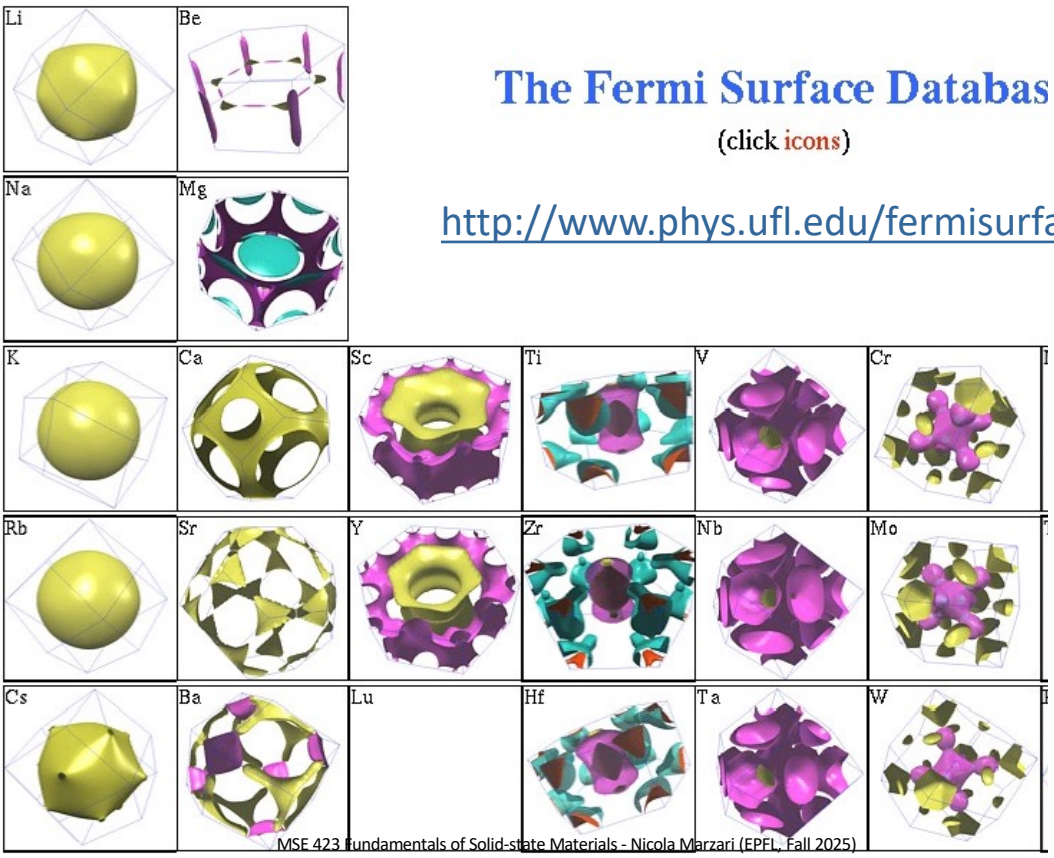
# The Fermi surface (fcc)




Cu






The Fermi Surface Databas

(click icons)

http://www.phys.ufl.edu/fermisurface/



# The independent-electron gas

- Hamiltonian

- Eigenvalues and eigenfunctions

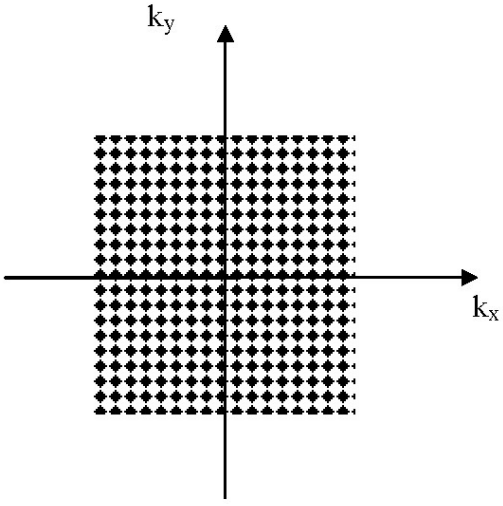
# The independent-electron gas

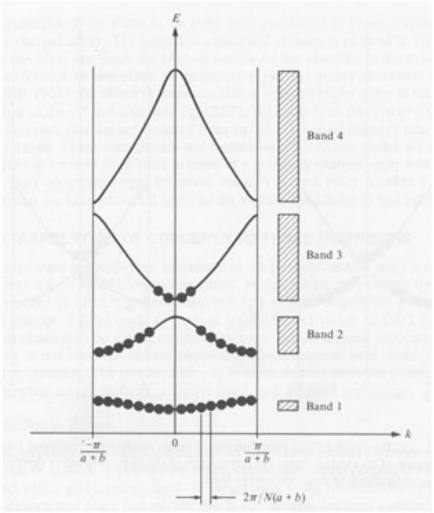
- BvK boundary conditions



# The independent-electron gas

- Counting the states



# The independent-electron gas

- Particle density



# The independent-electron gas

- Energy density