

MSE 423 Fall 2024 – Week 10

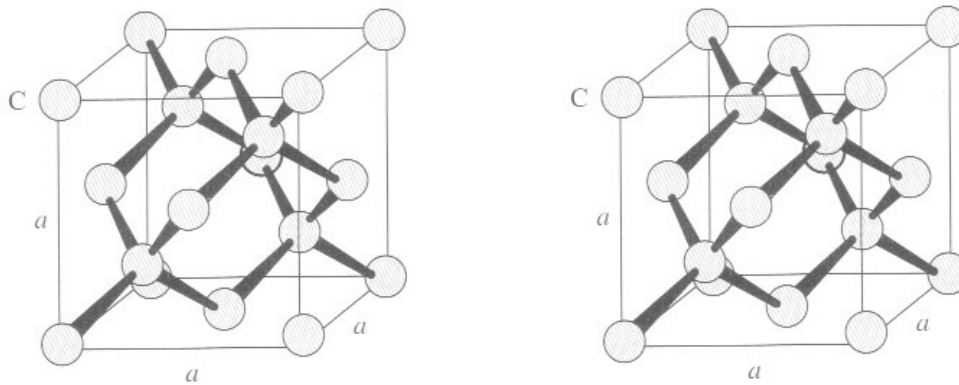


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Last week

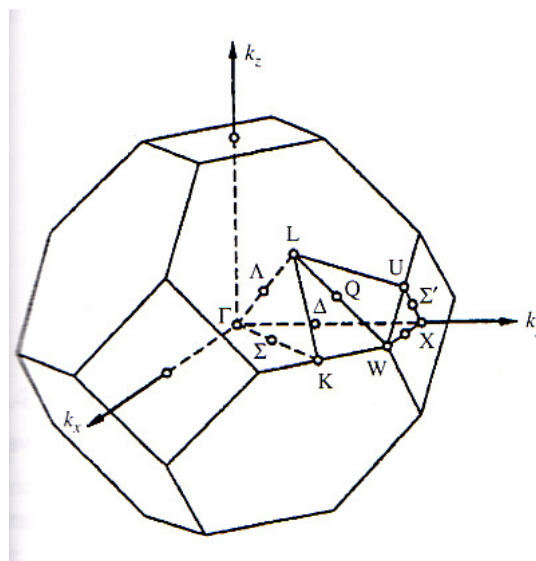
- Reciprocal lattice, and Brillouin zones
- Hamiltonian in a periodic potential, and graphical representation
- Bloch theorem, in two forms
- From k in extended space to 1st BZ + band index

Diamond and Zincblend



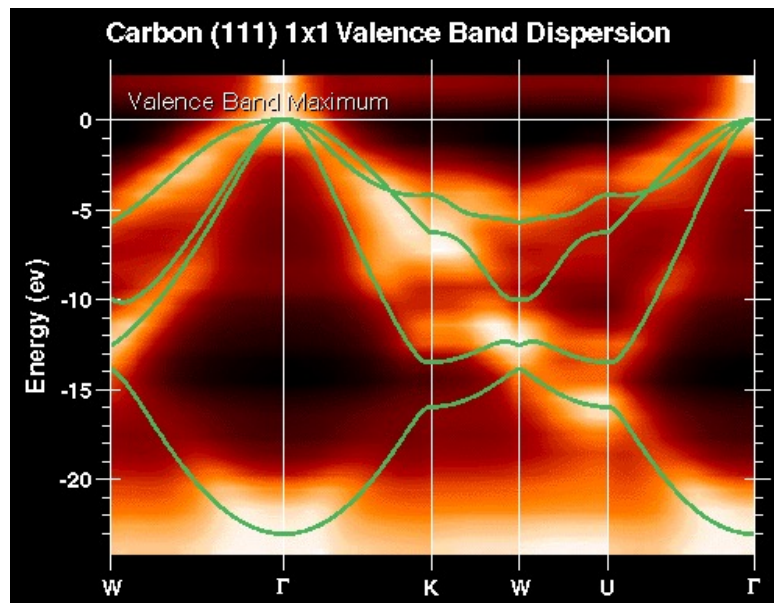
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Brillouin Zone (fcc)



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Band Structure of Diamond



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

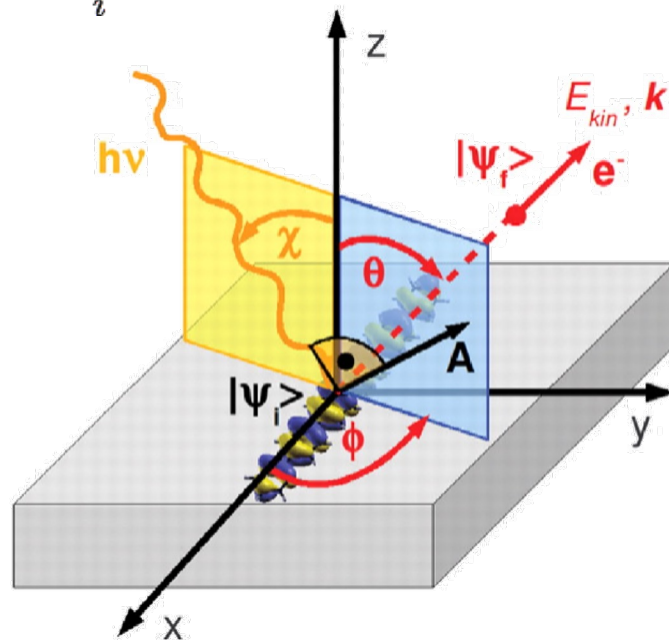
Section 2: Band Theory of Crystals

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

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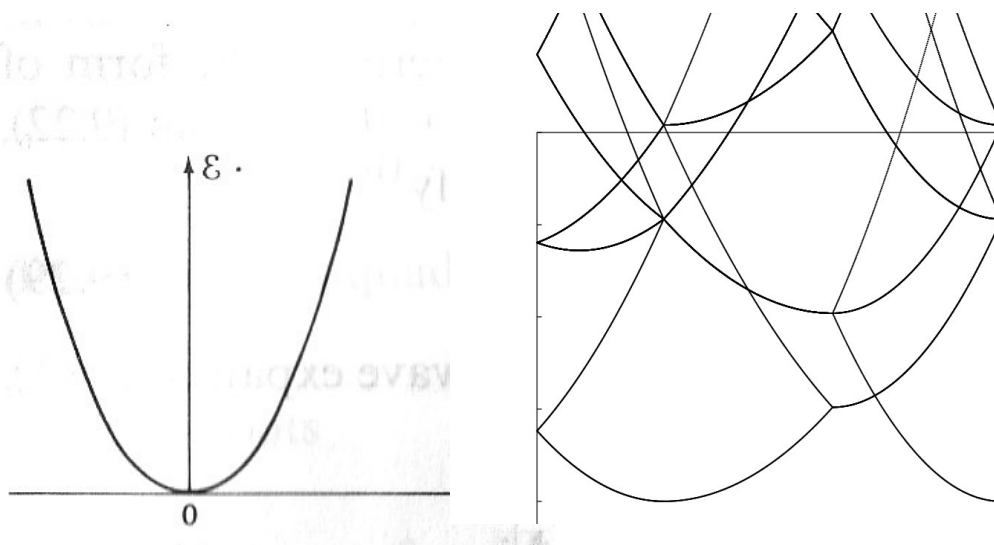
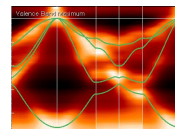
ARPES: Angle resolved photoemission spectroscopy

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



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Why does it look like this?



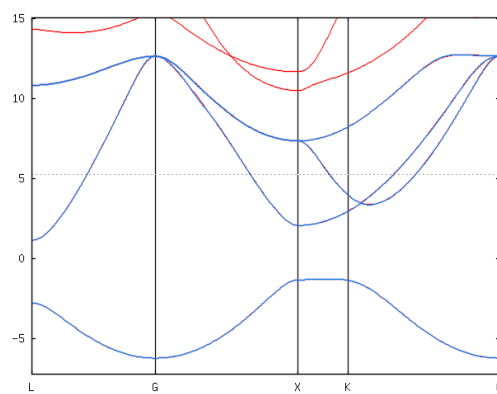
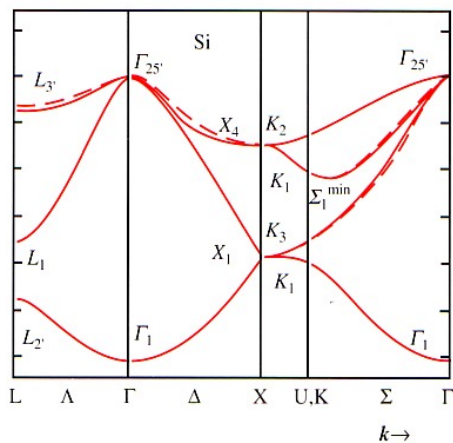
Band Structures: Free Electron Gas, Silicon



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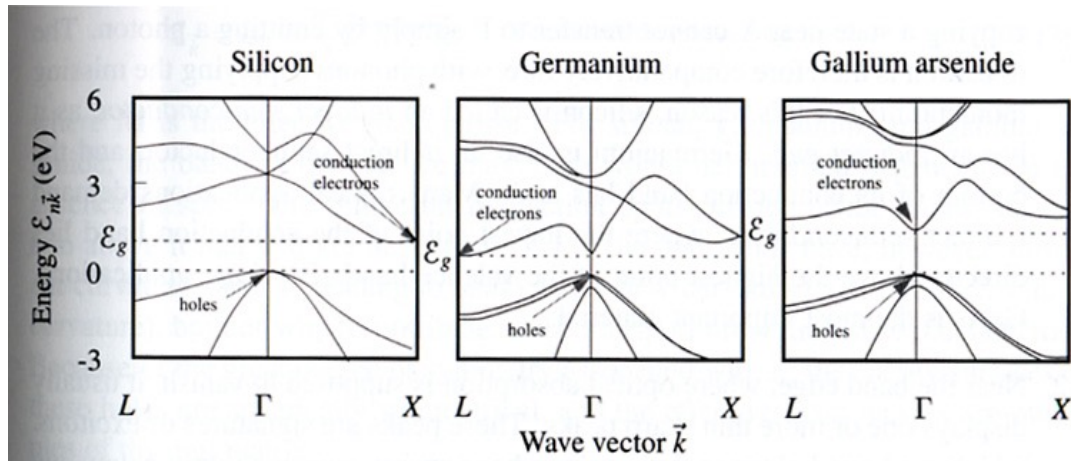
Silicon

Lead



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Band structure of Si, Ge, GaAs



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Conduction band minima (in 3d)

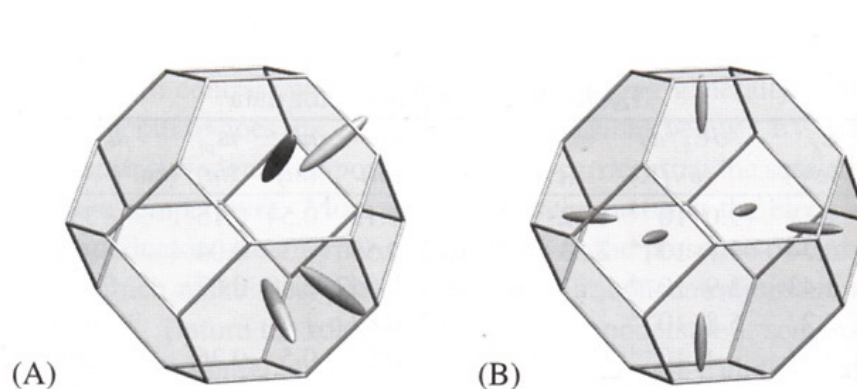


Figure 19.9. (A) The conduction band minima in germanium lie along (111) and straddle the zone boundary, producing four inequivalent pockets of electrons with a highly anisotropic effective mass. (B) In silicon, the conduction band minima lie 8/10 of the way toward (100) , producing six pockets of electrons,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

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Impress your examiners (orals)

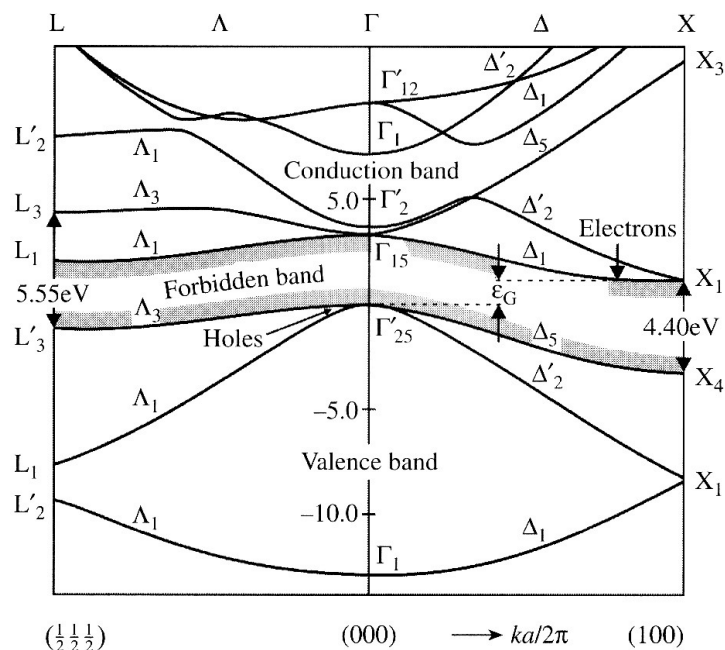
Table 19.1. Semiconductor data

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

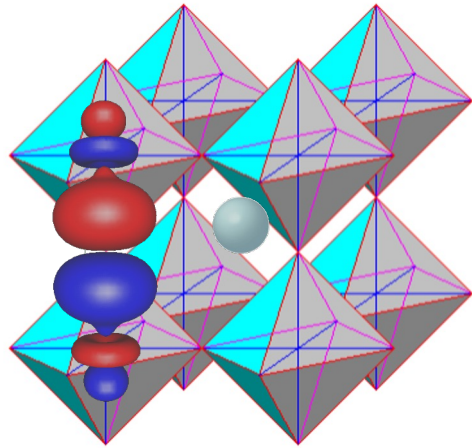
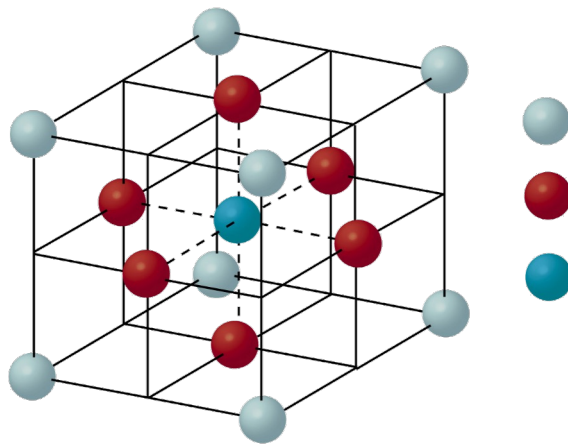
Data on whether a compound has a direct (d) or indirect (i) gap, energy gap, static dielectric constant, effective masses, and mobilities, for some semiconductors. The electron effective mass m_n^* is the density of states effective mass defined in Eq. (19.23). The data refer to room temperature, and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

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Valence+conduction bands in Si

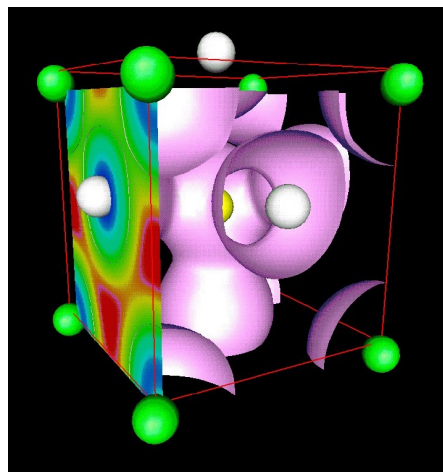
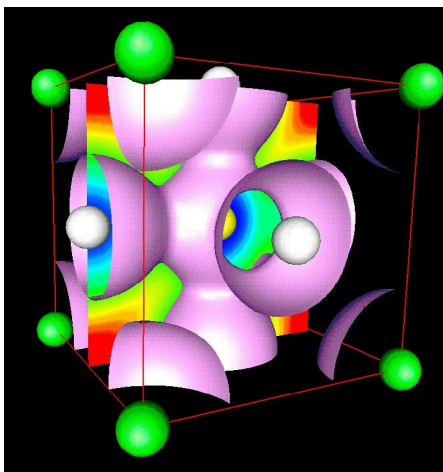


Perovskites



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Ferroelectric perovskites



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Ferroelectric perovskites

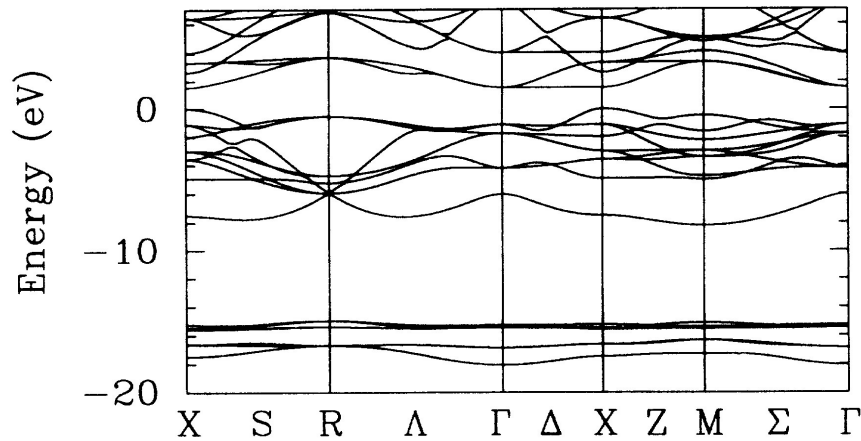
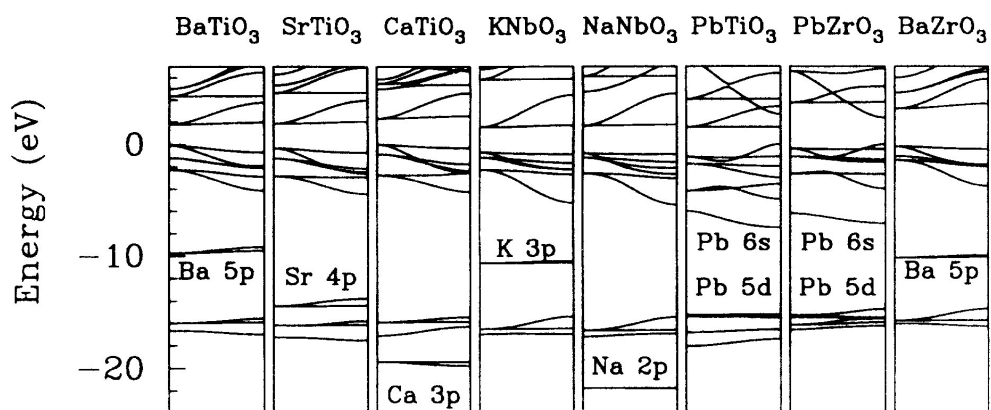


FIG. 3. Band structure of cubic PbTiO_3 for selected high-symmetry directions.

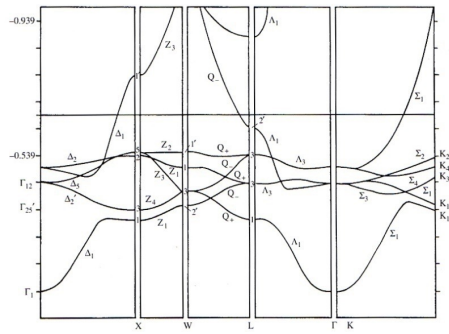
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Ferroelectric perovskites

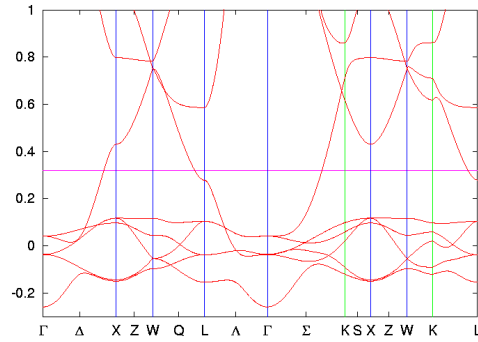


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Copper

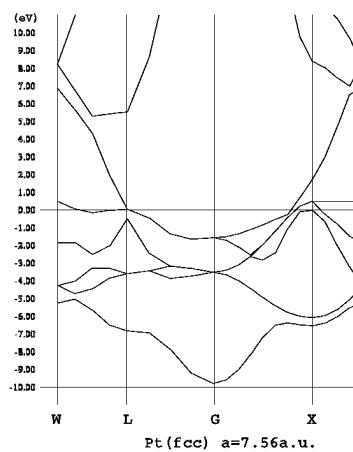


Silver

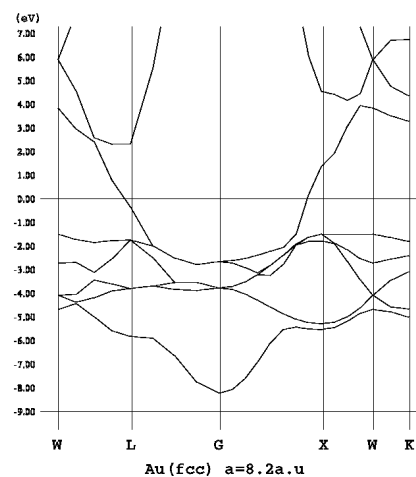


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Platinum



Gold

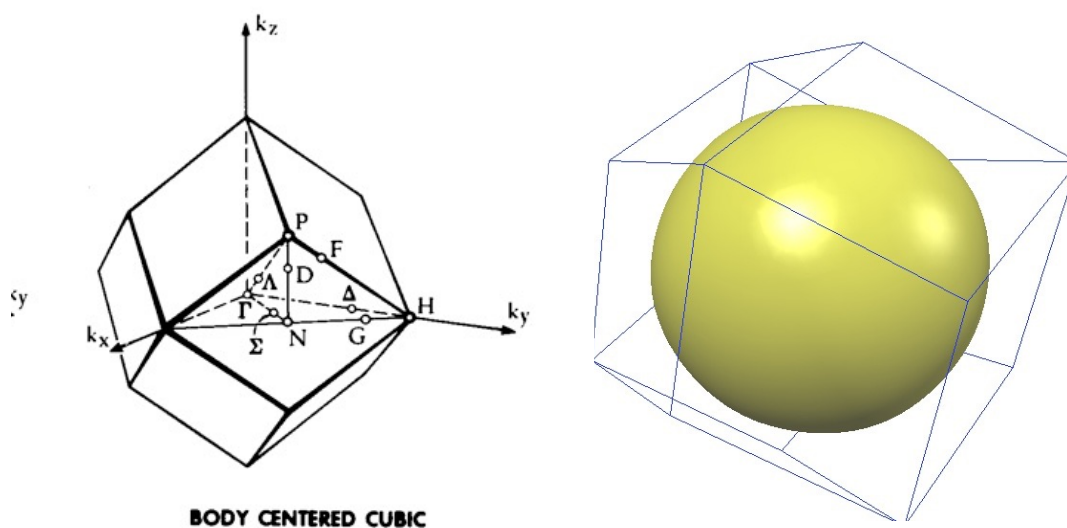


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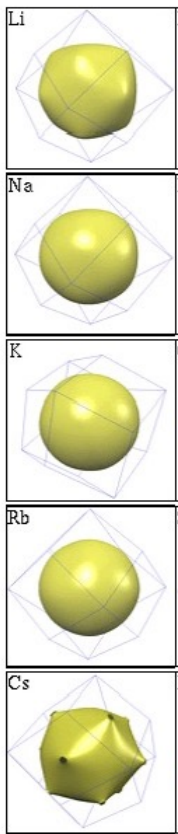
Group velocity, effective mass

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The Fermi surface

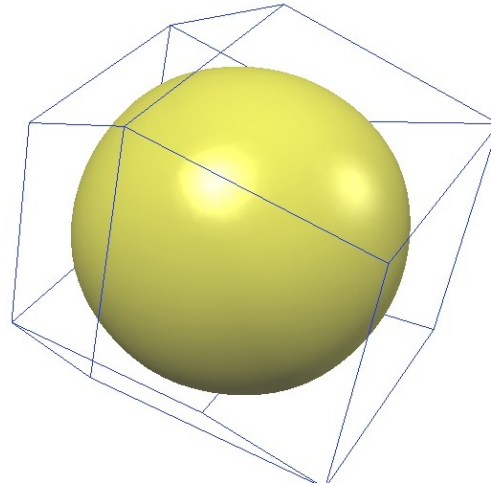


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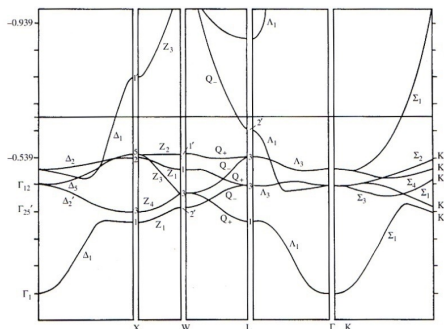
The Fermi surface

K

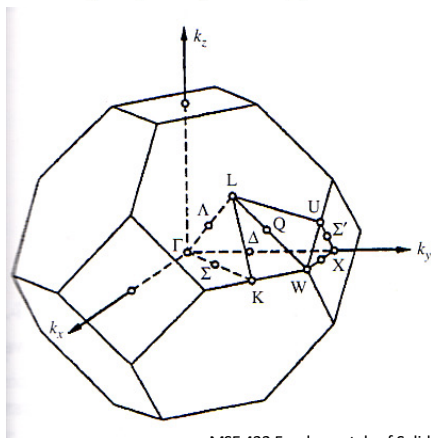
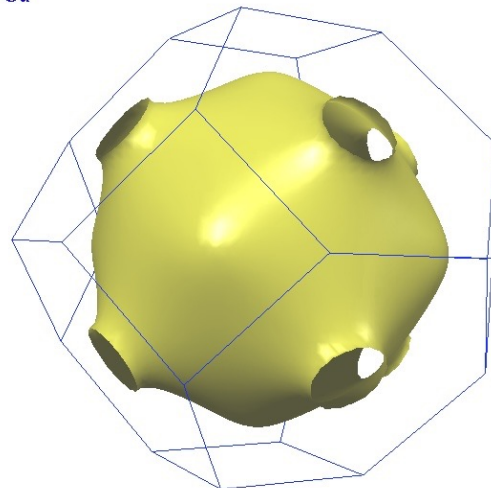


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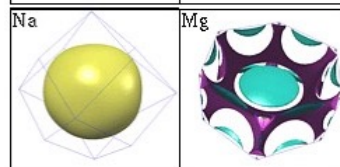
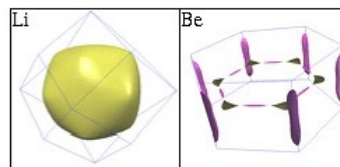
The Fermi surface (fcc)



Cu



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The Fermi Surface Databas

(click **icons**)

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

