Electron bands

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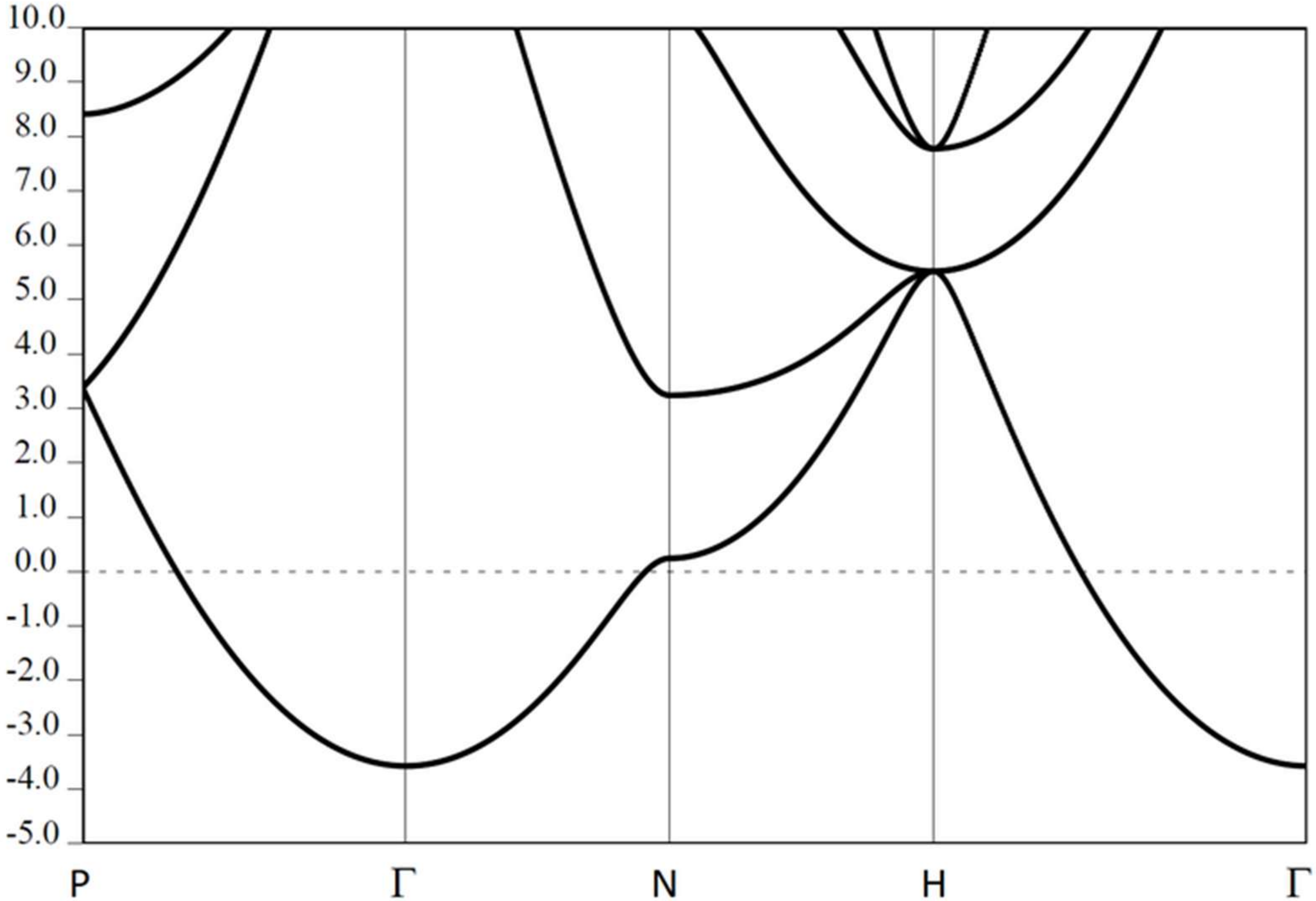
Band structures and Fermi surfaces of metallic elements

- Introduction
- Literature survey of calculations and experiments
- Data for Ac...Bi
- Data for C...Cu
- Data for Dy...Ir
- Data for K...Nd
- Data for Ni...Ru
- Data for Sb...Ti
- Data for Tl...Zr
- References

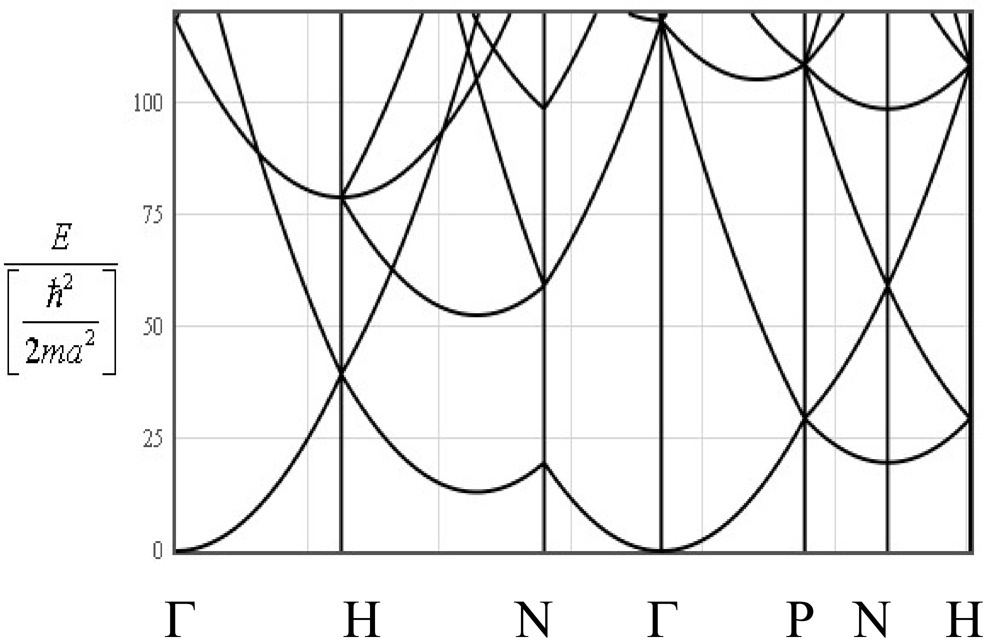
Density Functional Theory (DFT)

Bandstructure of bcc lithium (Li)

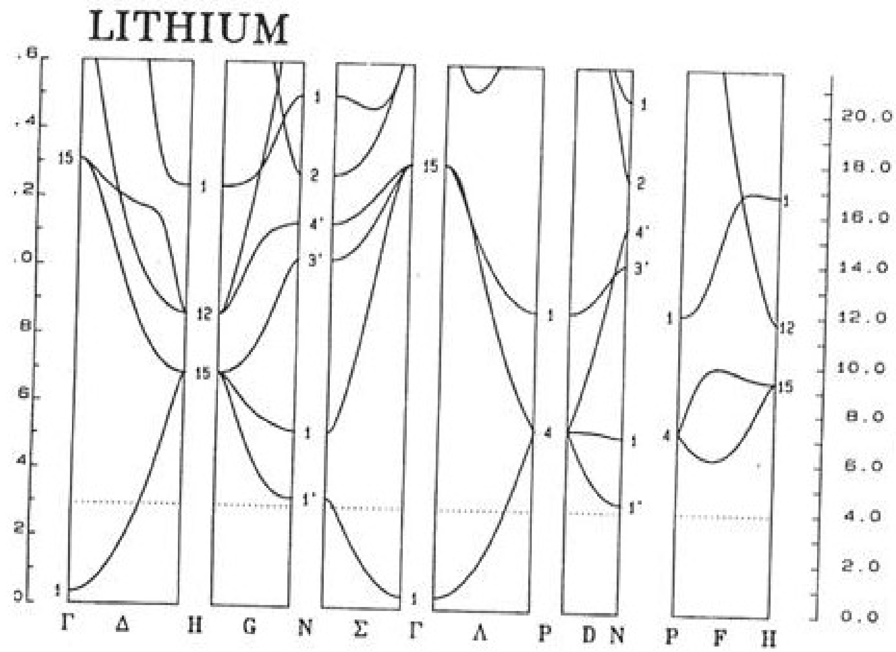


http://lampx.tugraz.at/~hadley/ss1/bands/bandstructures/Li/Li_Bandstructure.html

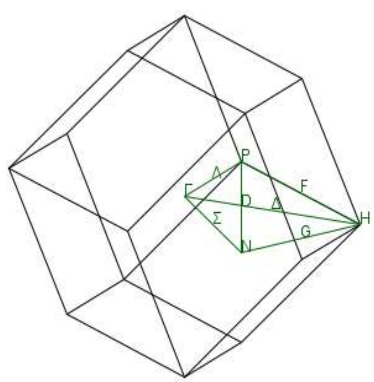
Lithium bcc



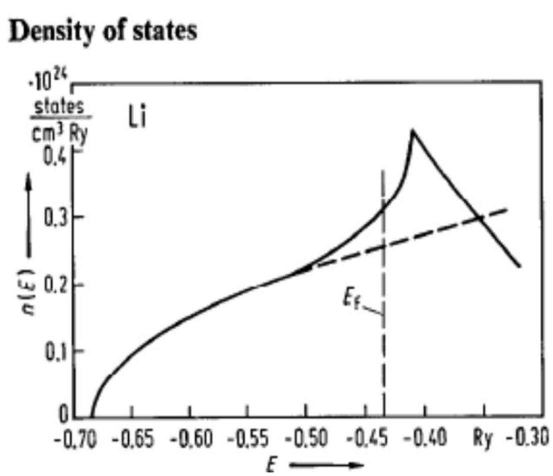
$\frac{E}{\left[\frac{\hbar^2}{2ma^2}\right]}$
0
25
50
75
100
Γ H N Γ P N H



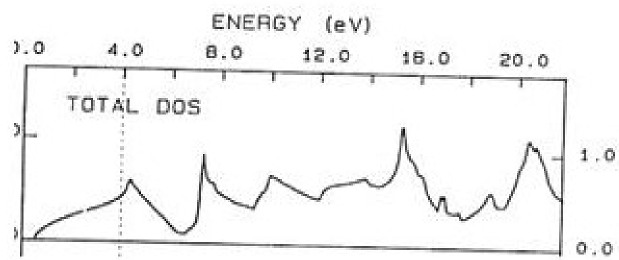
LITHIUM
Γ Δ H G N Σ Γ Λ P D N P F H



P
Λ
F
Γ
D
Δ
Σ
H
N
G

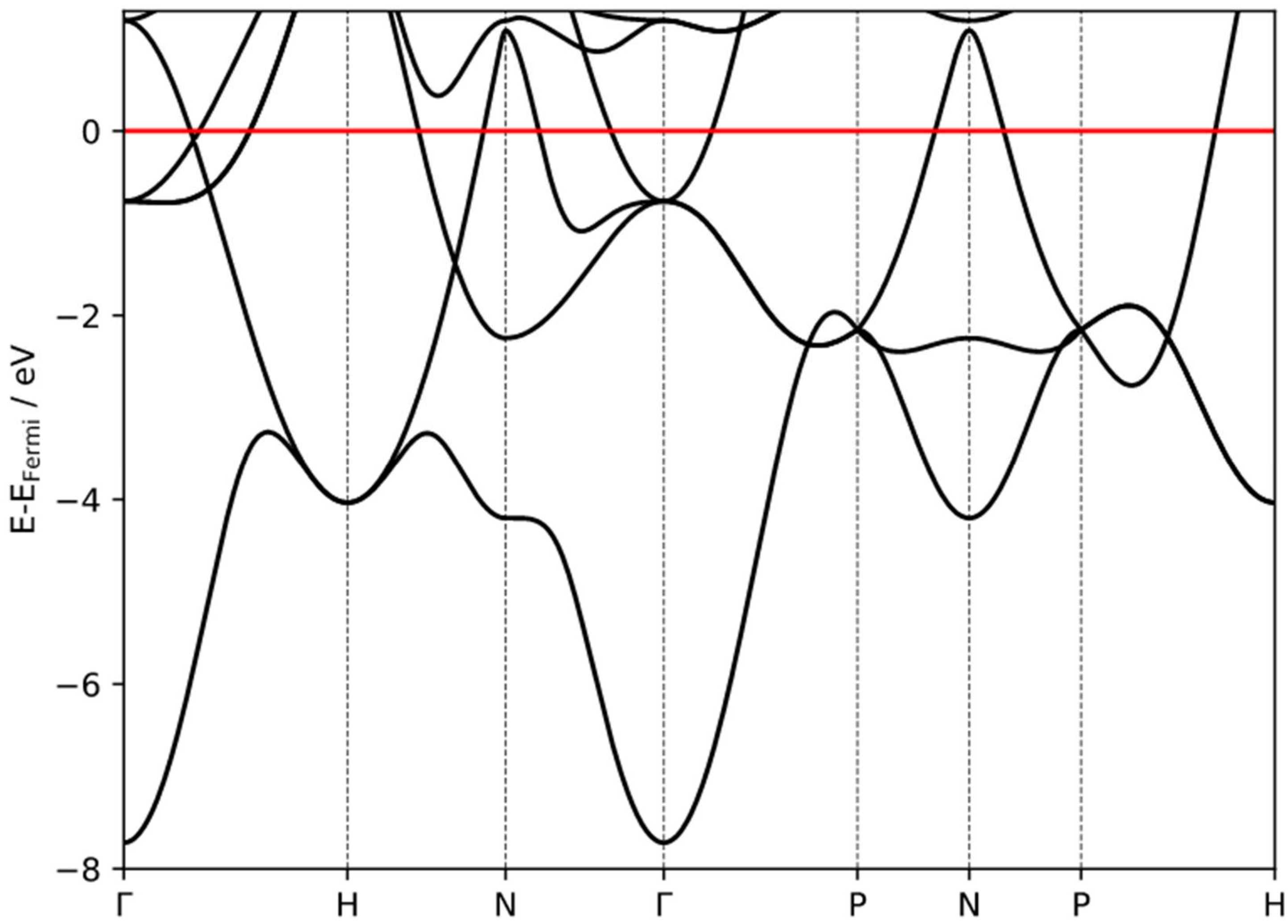


Density of states
$\cdot 10^{24}$ states / cm³ Ry
Li
n(E)
E_F
Ry
E



ENERGY (eV)
TOTAL DOS

Bandstructure of bcc chromium (Cr)



http://lampx.tugraz.at/~hadley/ss1/bands/bandstructures/Cr/Cr_Bandstructure.html

Sodium

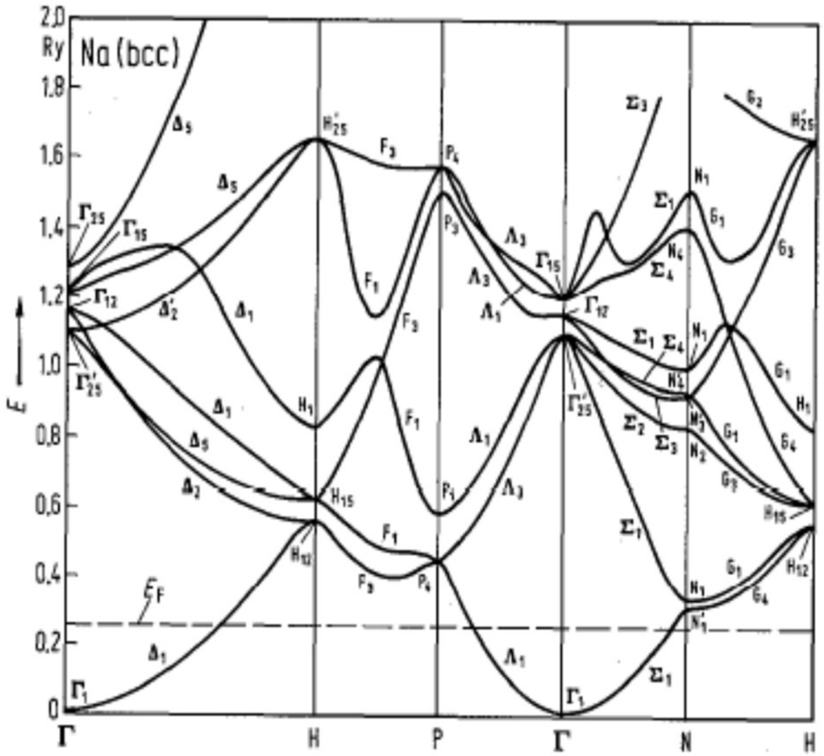
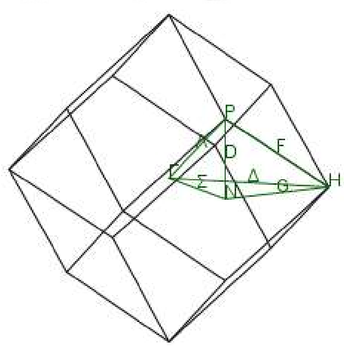
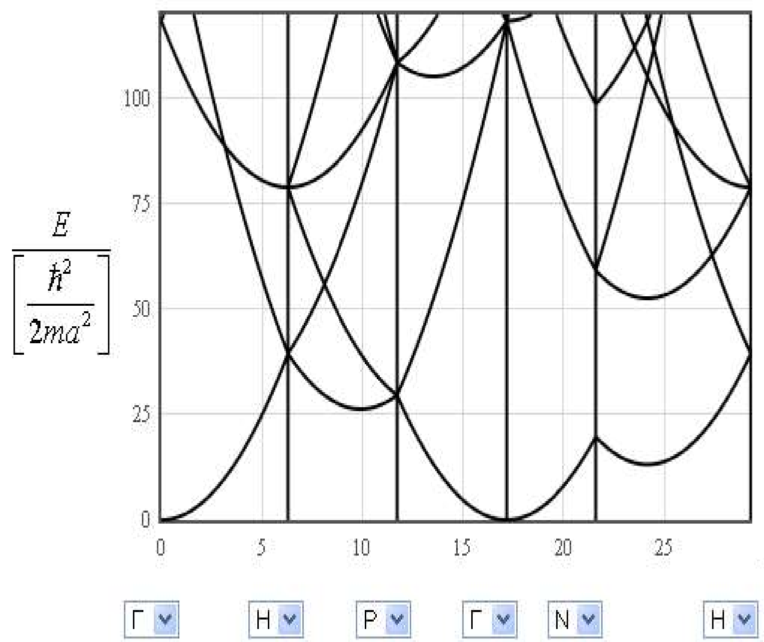
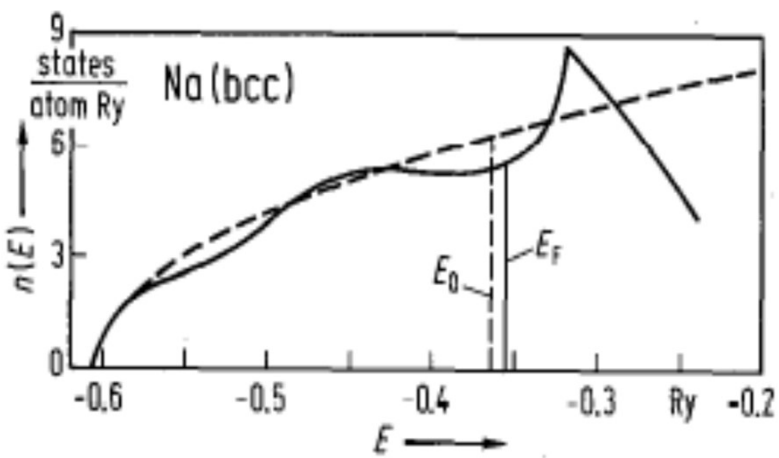


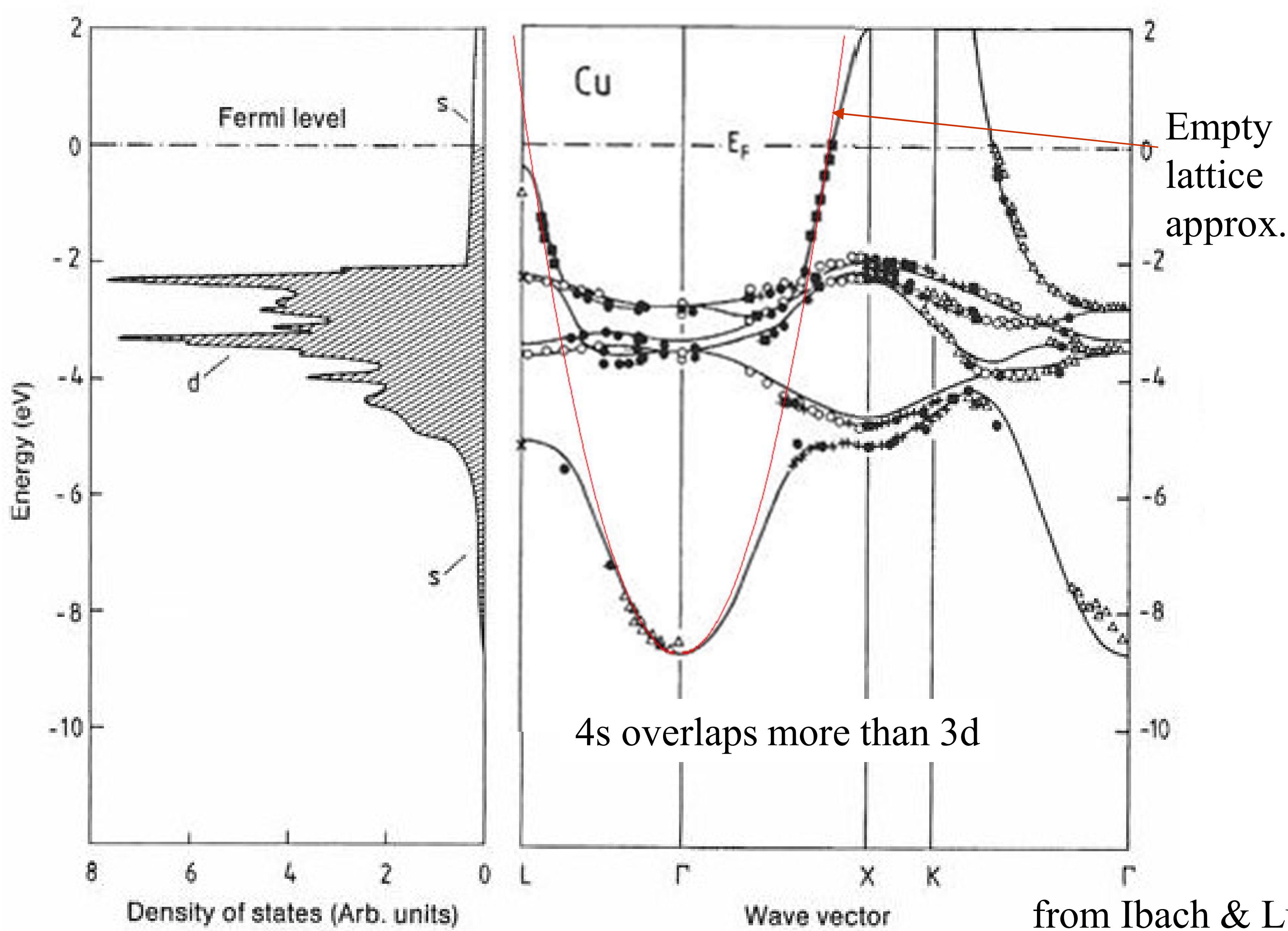
Fig. 6. Na (bcc). Energy bands calculated using the APW method by Gupta (quoted in [73Haq]).







Copper dispersion relation and density of states



from Ibach & Lueth

Silver

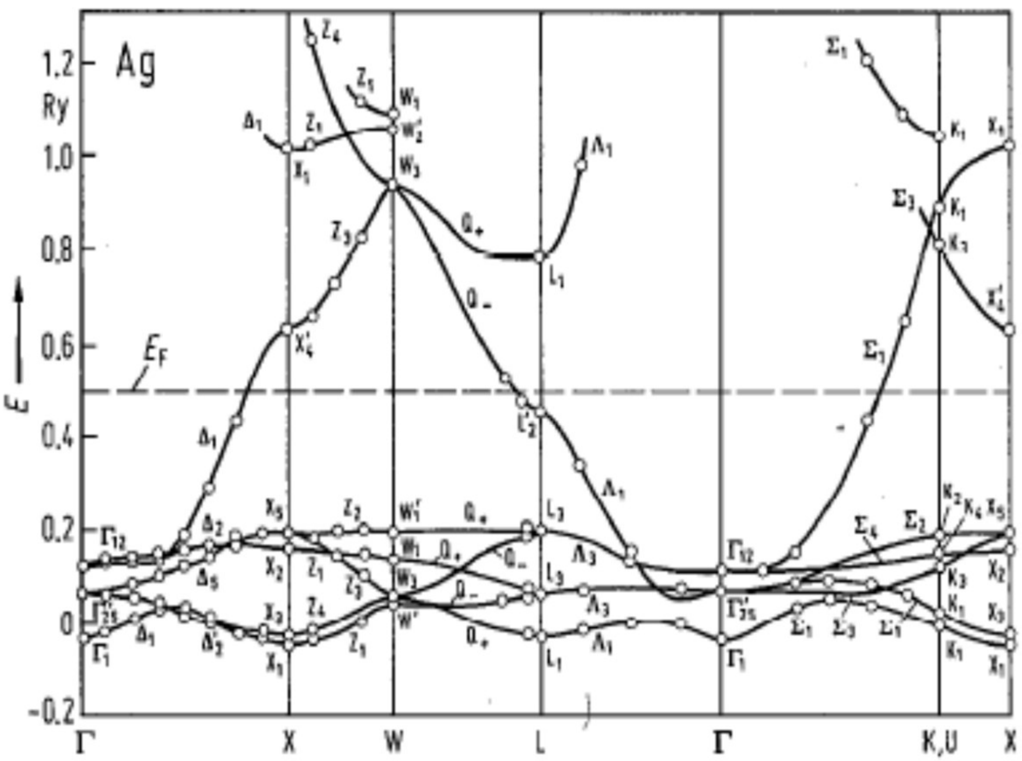


Fig. 3. Ag. Energy bands calculated using the APW method [69Chr].

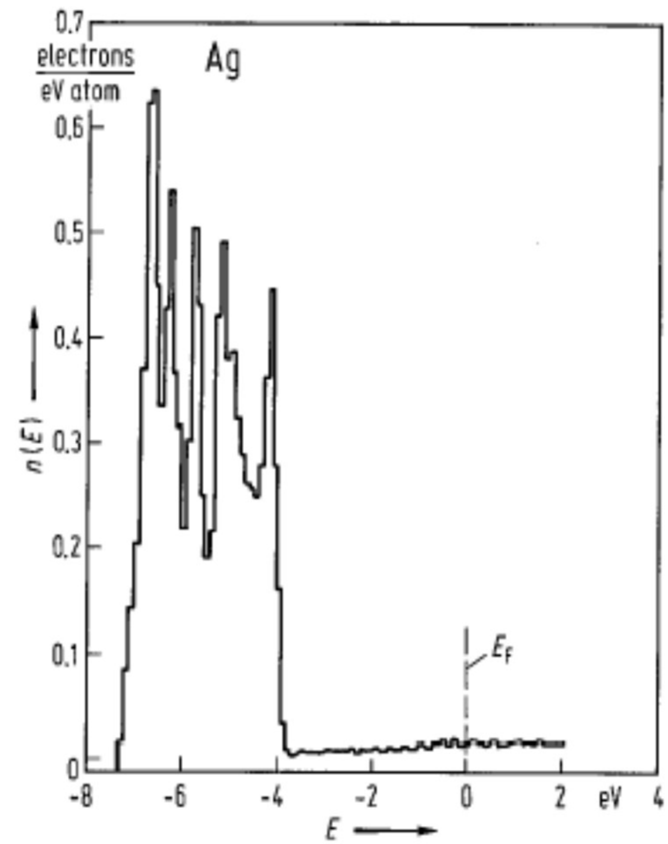
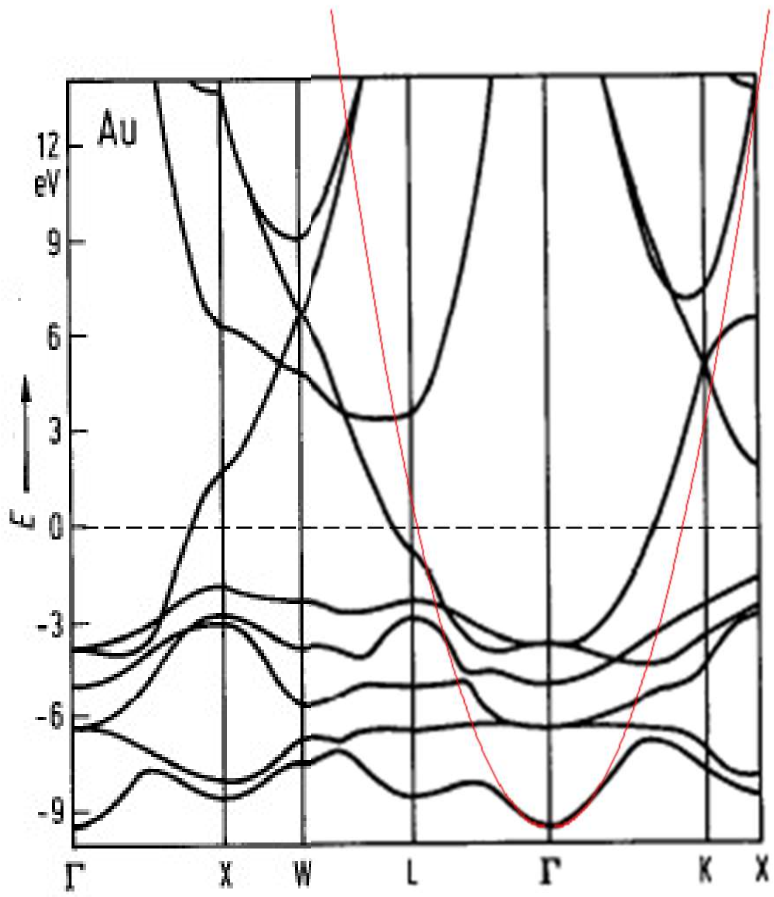


Fig. 15. Ag. Density of states calculated from the energy bands in Fig. 10. Ag [75Fon].

Gold



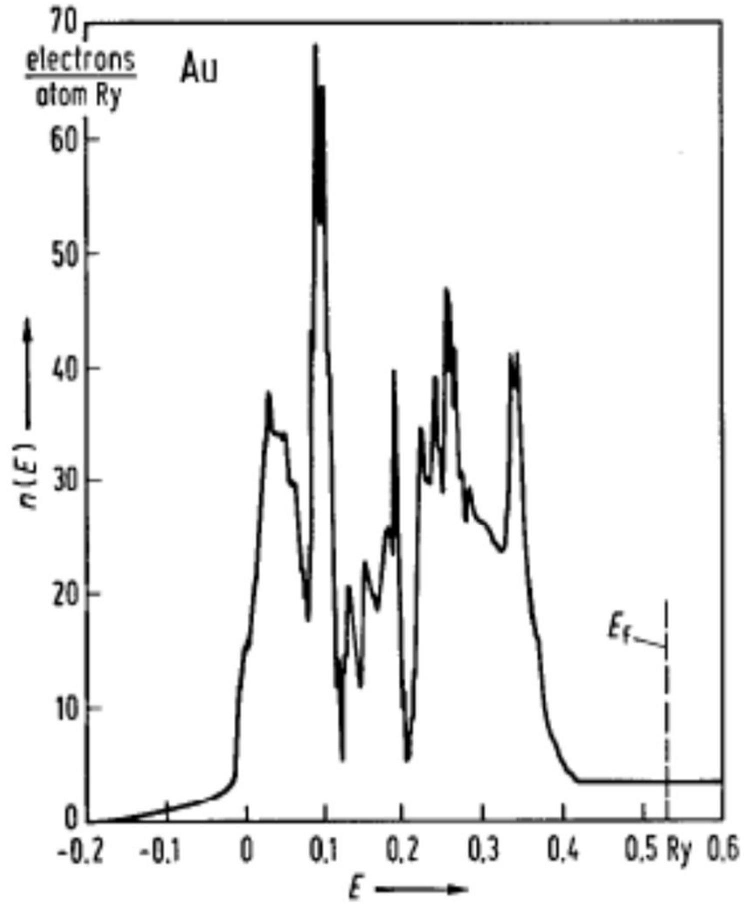


Fig. 9. Au. Density of states calculated from the energy bands in Fig. 4b. Au [71Chr2].

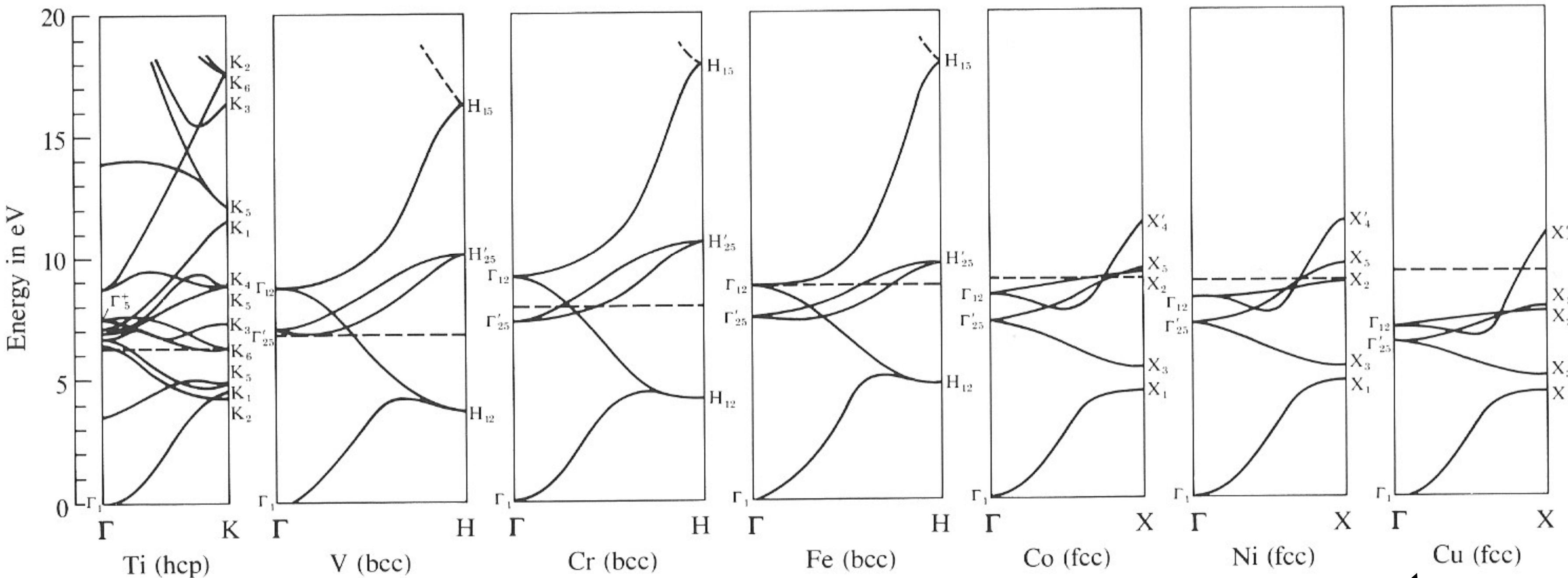
hydrogen 1 H 1.0079																		helium 2 He 4.0026
lithium 3 Li 6.941	beryllium 4 Be 9.0122												boron 5 B 10.811	carbon 6 C 12.011	nitrogen 7 N 14.007	oxygen 8 O 15.999	fluorine 9 F 18.998	neon 10 Ne 20.180
sodium 11 Na 22.990	magnesium 12 Mg 24.305												aluminium 13 Al 26.982	silicon 14 Si 28.086	phosphorus 15 P 30.974	sulfur 16 S 32.065	chlorine 17 Cl 35.453	argon 18 Ar 39.948
potassium 19 K 39.098	calcium 20 Ca 40.078		scandium 21 Sc 44.956	titanium 22 Ti 47.867	vanadium 23 V 50.942	chromium 24 Cr 51.996	manganese 25 Mn 54.938	iron 26 Fe 55.845	cobalt 27 Co 58.933	nickel 28 Ni 58.693	copper 29 Cu 63.546	zinc 30 Zn 65.39	gallium 31 Ga 69.723	germanium 32 Ge 72.61	arsenic 33 As 74.922	selenium 34 Se 78.96	bromine 35 Br 79.904	krypton 36 Kr 83.80
rubidium 37 Rb 85.468	strontium 38 Sr 87.62		yttrium 39 Y 88.906	zirconium 40 Zr 91.224	niobium 41 Nb 92.906	molybdenum 42 Mo 95.94	technetium 43 Tc [98]	ruthenium 44 Ru 101.07	rhodium 45 Rh 102.91	palladium 46 Pd 106.42	silver 47 Ag 107.87	cadmium 48 Cd 112.41	indium 49 In 114.82	tin 50 Sn 118.71	antimony 51 Sb 121.76	tellurium 52 Te 127.60	iodine 53 I 126.90	xenon 54 Xe 131.29
caesium 55 Cs 132.91	barium 56 Ba 137.33	57-70 *	lutetium 71 Lu 174.97	hafnium 72 Hf 178.49	tantalum 73 Ta 180.95	tungsten 74 W 183.84	rhenium 75 Re 186.21	osmium 76 Os 190.23	iridium 77 Ir 192.22	platinum 78 Pt 195.08	gold 79 Au 196.97	mercury 80 Hg 200.59	thallium 81 Tl 204.38	lead 82 Pb 207.2	bismuth 83 Bi 208.98	polonium 84 Po [209]	astatine 85 At [210]	radon 86 Rn [222]
francium 87 Fr [223]	radium 88 Ra [226]	89-102 **	lawrencium 103 Lr [262]	rutherfordium 104 Rf [261]	dubnium 105 Db [262]	seaborgium 106 Sg [266]	bohrium 107 Bh [264]	hassium 108 Hs [269]	meitnerium 109 Mt [268]	ununnilium 110 Uun [271]	unununium 111 Uuu [272]	ununbium 112 Uub [277]		ununquadium 114 Uuq [289]				

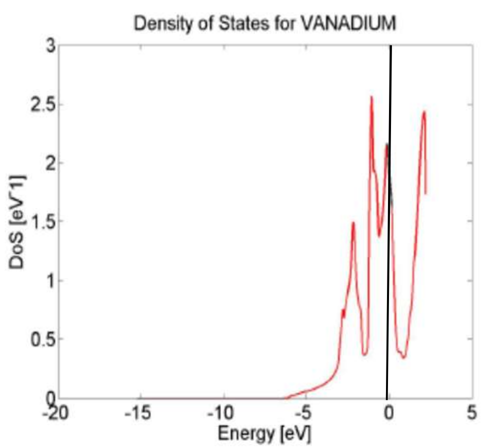
d band metals, transition metals

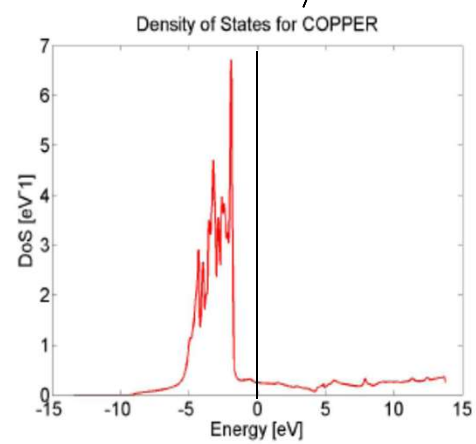
*Lanthanide series	lanthanum 57 La 138.91	cerium 58 Ce 140.12	praseodymium 59 Pr 140.91	neodymium 60 Nd 144.24	promethium 61 Pm [145]	samarium 62 Sm 150.36	europium 63 Eu 151.96	gadolinium 64 Gd 157.25	terbium 65 Tb 158.93	dysprosium 66 Dy 162.50	holmium 67 Ho 164.93	erbium 68 Er 167.26	thulium 69 Tm 168.93	ytterbium 70 Yb 173.04
**Actinide series	actinium 89 Ac [227]	thorium 90 Th 232.04	protactinium 91 Pa 231.04	uranium 92 U 238.03	neptunium 93 Np [237]	plutonium 94 Pu [244]	americium 95 Am [243]	curium 96 Cm [247]	berkelium 97 Bk [247]	californium 98 Cf [251]	einsteinium 99 Es [252]	fermium 100 Fm [257]	mendelevium 101 Md [258]	nobelium 102 No [259]

f band metals, rare earths

Transition metals



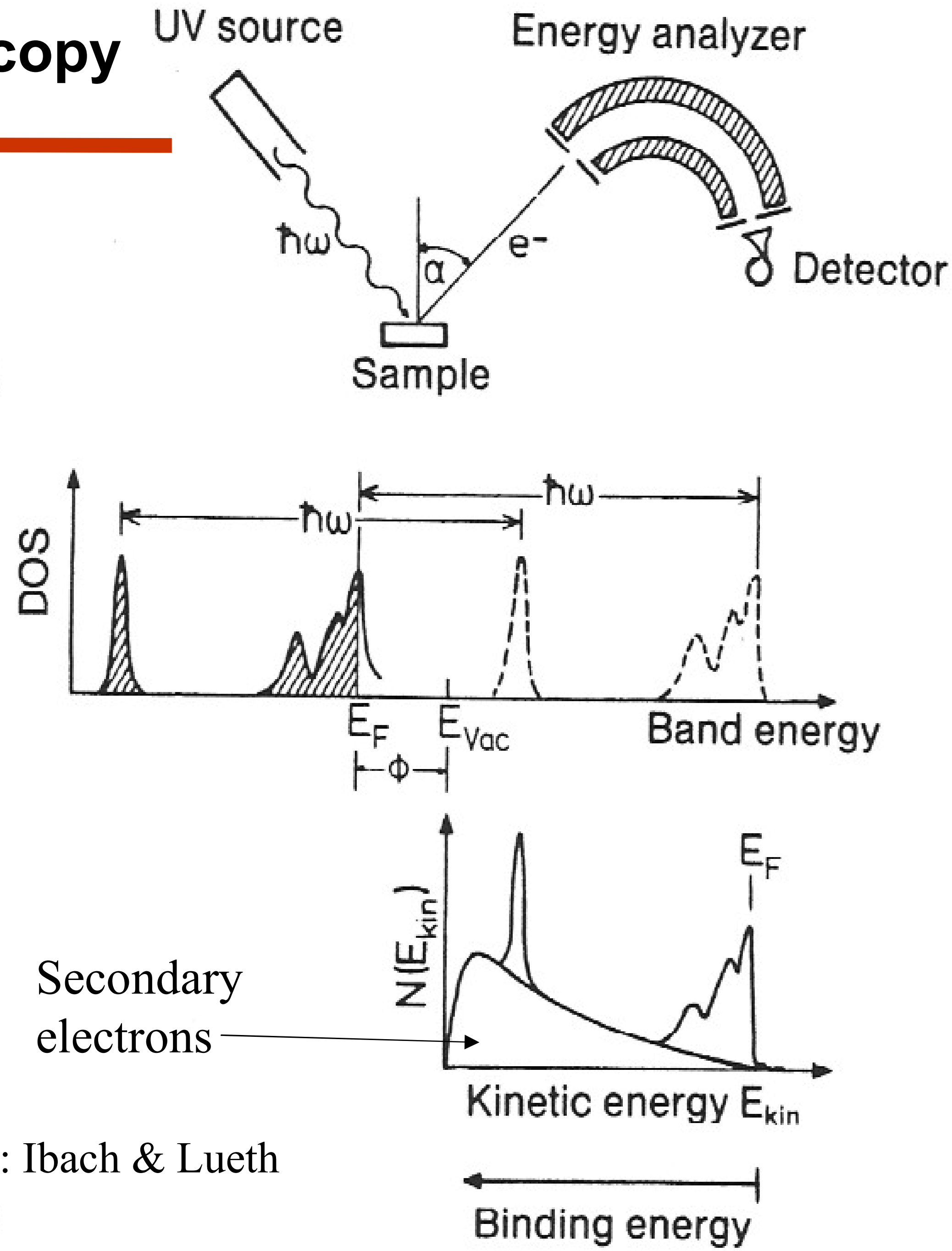




Photoemission spectroscopy

UPS - Ultraviolet
photoemission spectroscopy

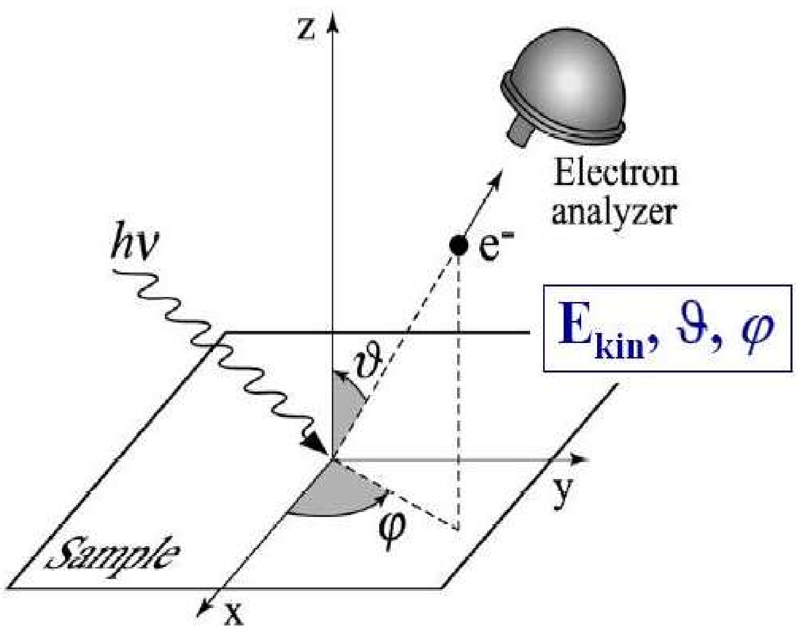
Measure the density of states with photoemission spectroscopy

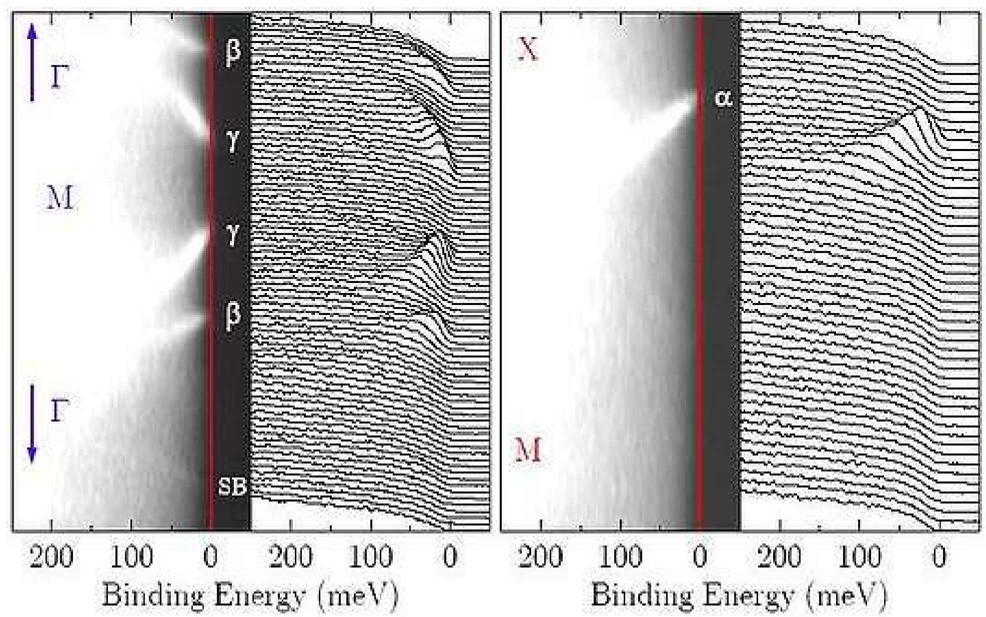


Secondary electrons

From: Ibach & Lueth

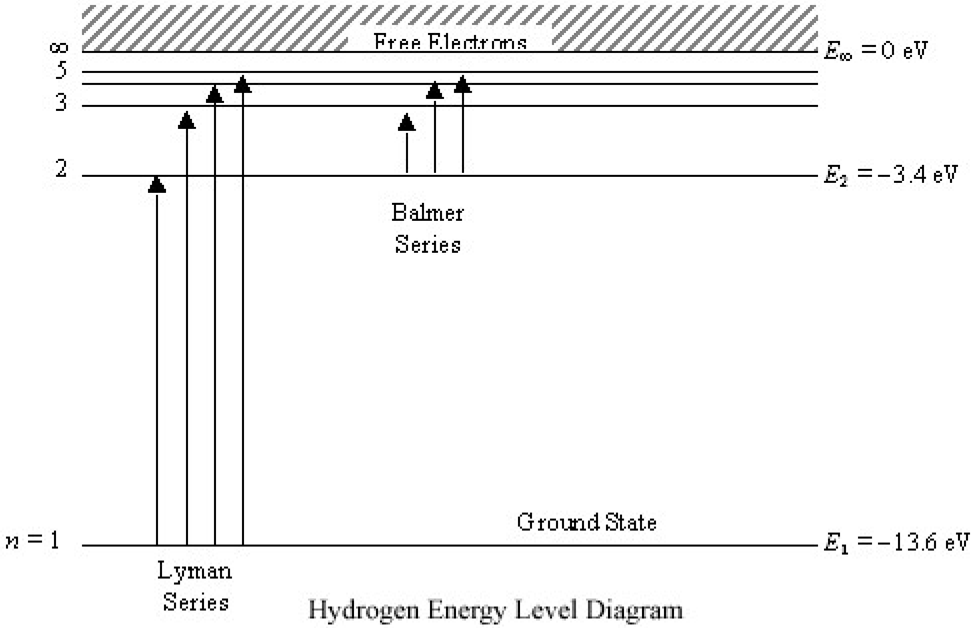
Angle resolved photoemission spectroscopy (ARPES)



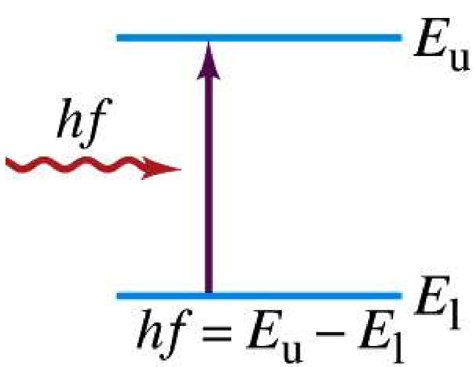


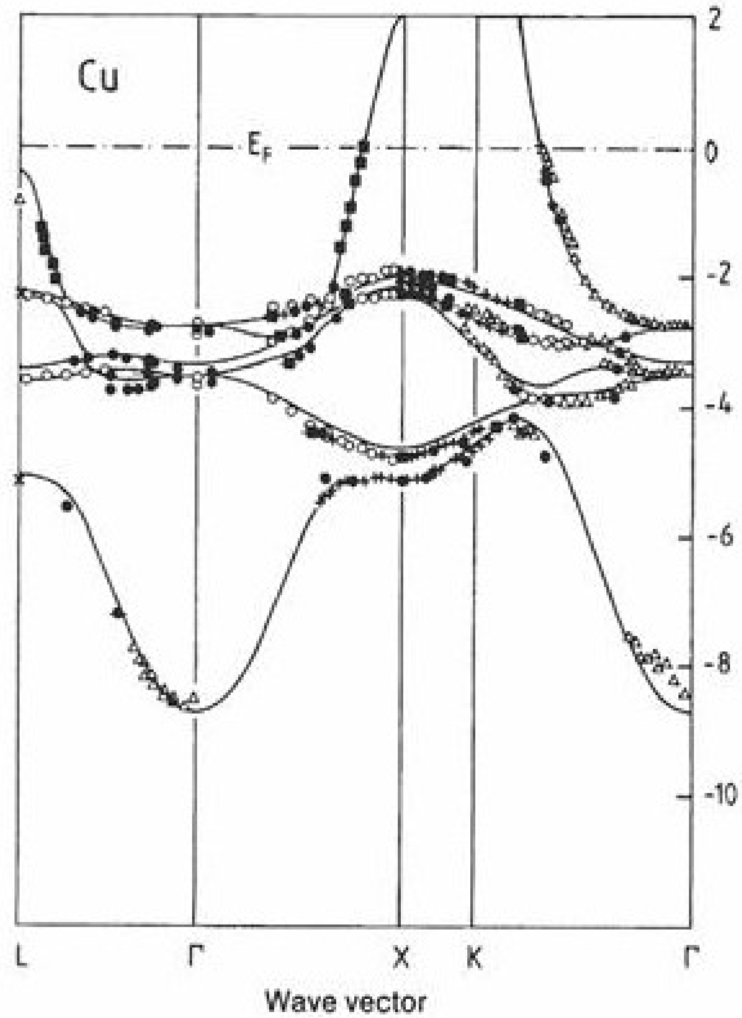
Measure the dispersion relation with angle resolved photoemission

Optical absorption



Hydrogen atom



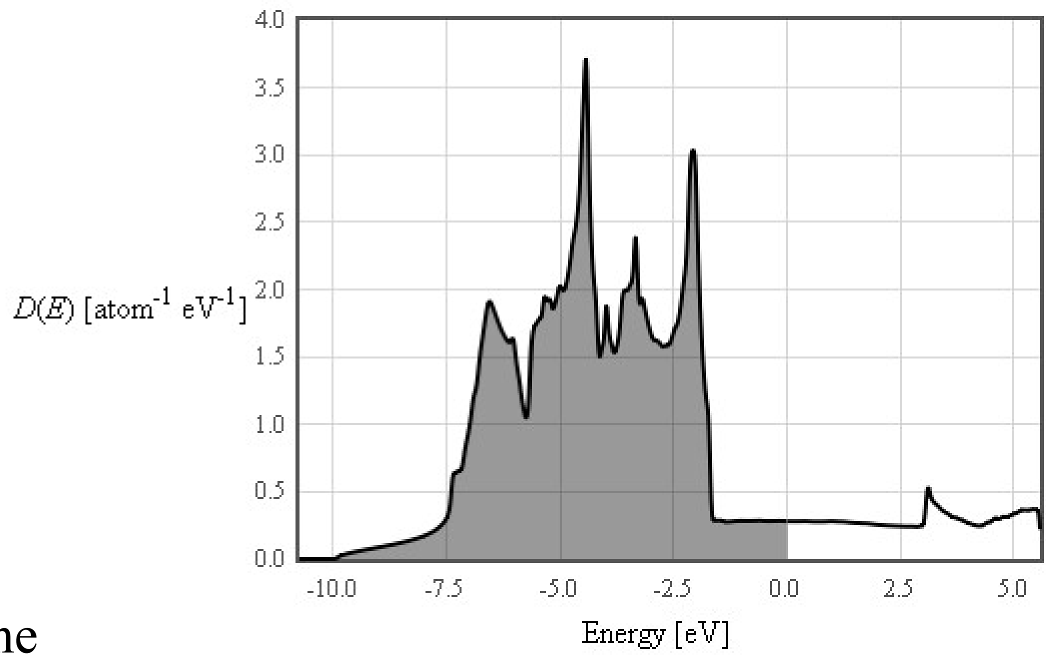


Copper fcc crystal

Thermodynamic properties of metals

From the band structure measurements, we obtain the electron density of states.

Electron density of states for fcc gold



E [eV]	$D(E)$ [atom^{-1} eV^{-1}]
-10.74913	0
-10.73552	0
-10.72192	0

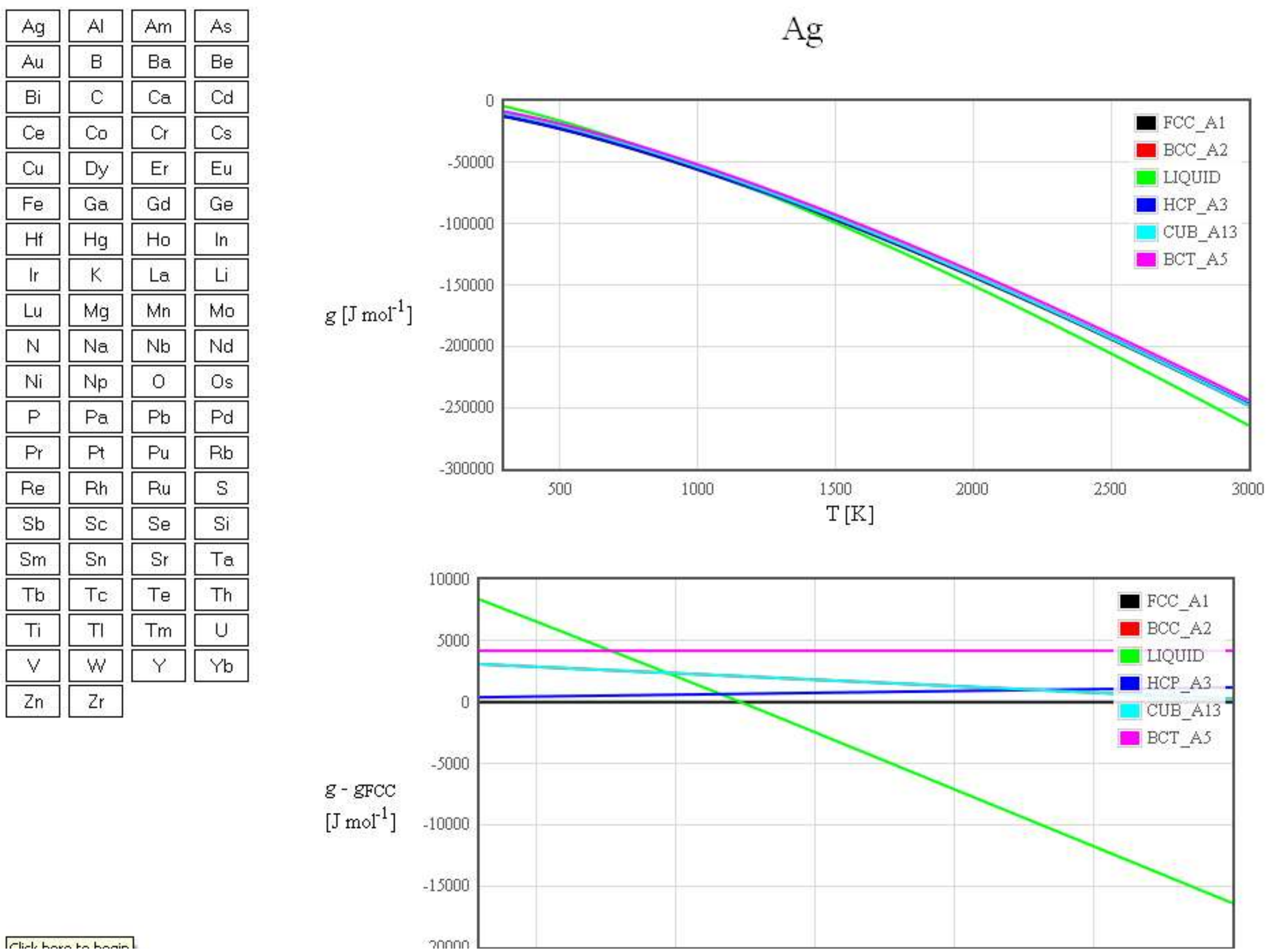
Thermodynamic properties can be calculated from the tabulated data for the density of states

SGTE data for pure elements

SGTE thermodynamic data

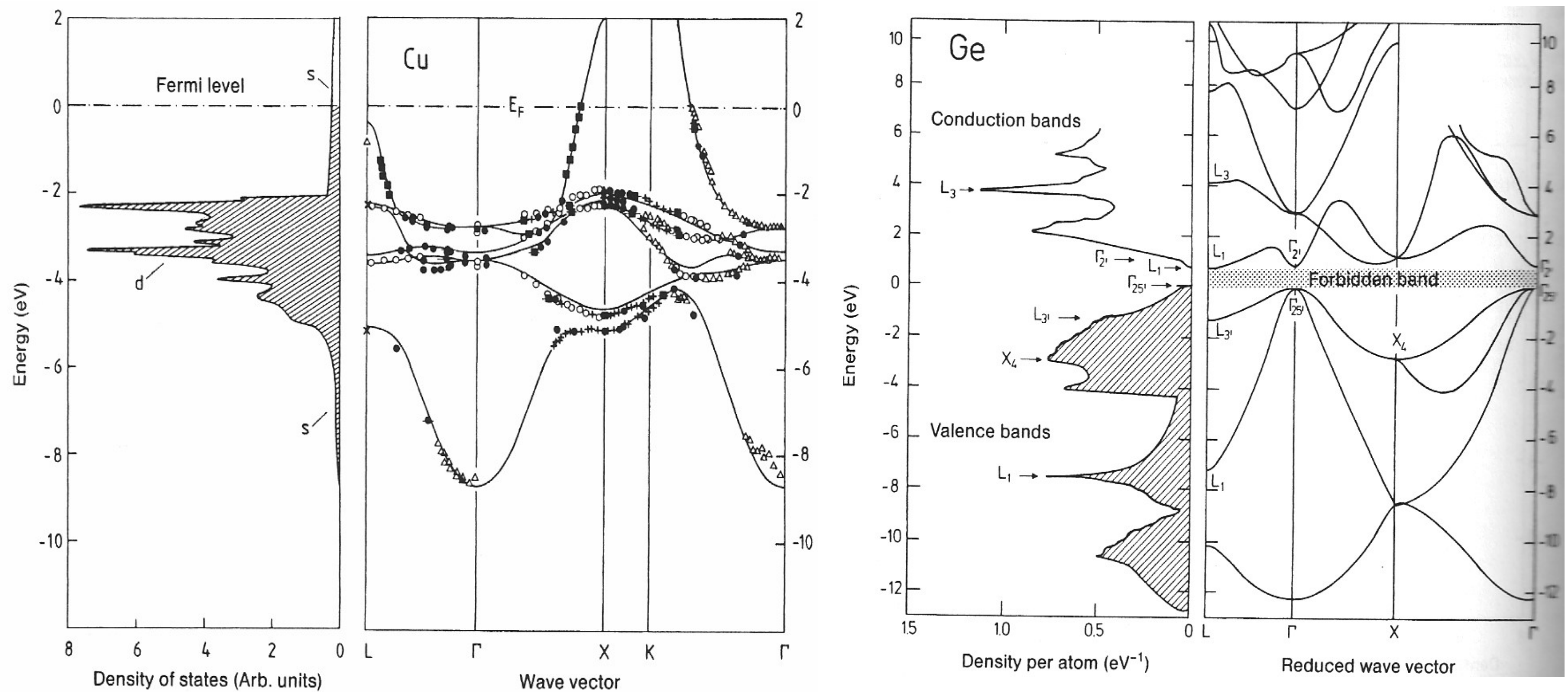
The Scientific Group Thermodata Europe SGTE maintains thermodynamic databanks for inorganic and metallurgical systems. Data from their 'pure element database' is plotted below.

Typically, experiments are performed at constant pressure p, temperature T, and number N. Under these conditions, the system will go to the minimum of the Gibbs energy $G = U + pV - TS$. Here U is the internal energy, V is the volume, and S is the entropy. The top plot is the Gibbs energy per mole $g = u + pv - Ts$, where u is the internal energy per mole, v is the volume per mole, and s is the entropy per mole.



http://www.sciencedirect.com/science/article/pii/036459169190030N

Metals, semiconductors, and insulators



Insulators: band gap > 3 eV

From Ibach & Lueth

Student Projects

Plot the dispersion relation for a 1-D square wave potential
Using the Kronig-Penney model, the plane wave method, and tight binding.

Draw the missing Fermi surfaces

Use the tight-binding model to calculate a dispersion relation.

Expand the table of tight binding solutions and
plane wave method solutions

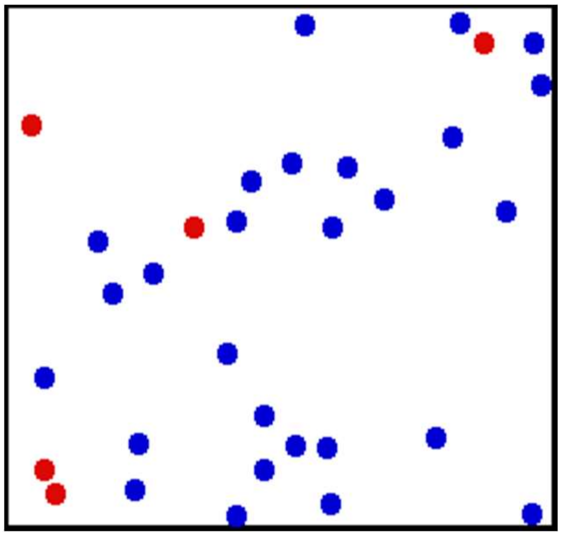
kinetic theory

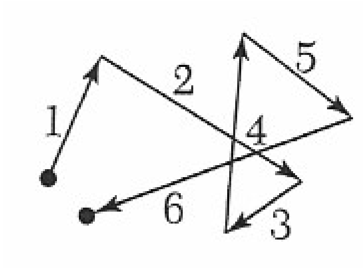
describe electrons as a gas of particles

$v_F = 10^8$ cm/s.

The average time between scattering events τ_{sc} can be calculated by Fermi's golden rule

mean free path: $\boldsymbol{l} = v_F \tau_{sc}$ ~ 1 nm - 1 cm





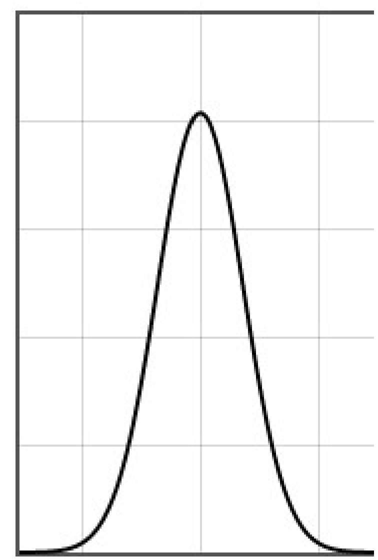
Diffusion equation/ heat equation

$$\frac{dn}{dt} = -D\nabla^2 n$$

Diffusion constant

Fick's law $\qquad \vec{j} = -D\nabla n$

Continuity equation $\qquad \frac{dn}{dt} = \nabla \cdot \vec{j}$



$$n = \frac{1}{\sqrt{4\pi Dt}} \exp\left(\frac{-r^2}{4Dt}\right)$$

Ballistic transport

$$\vec{F} = m\vec{a} = -e\vec{E} = m\frac{d\vec{v}}{dt}$$

$$\vec{v} = \frac{-e\vec{E}t}{m} + \vec{v}_0$$

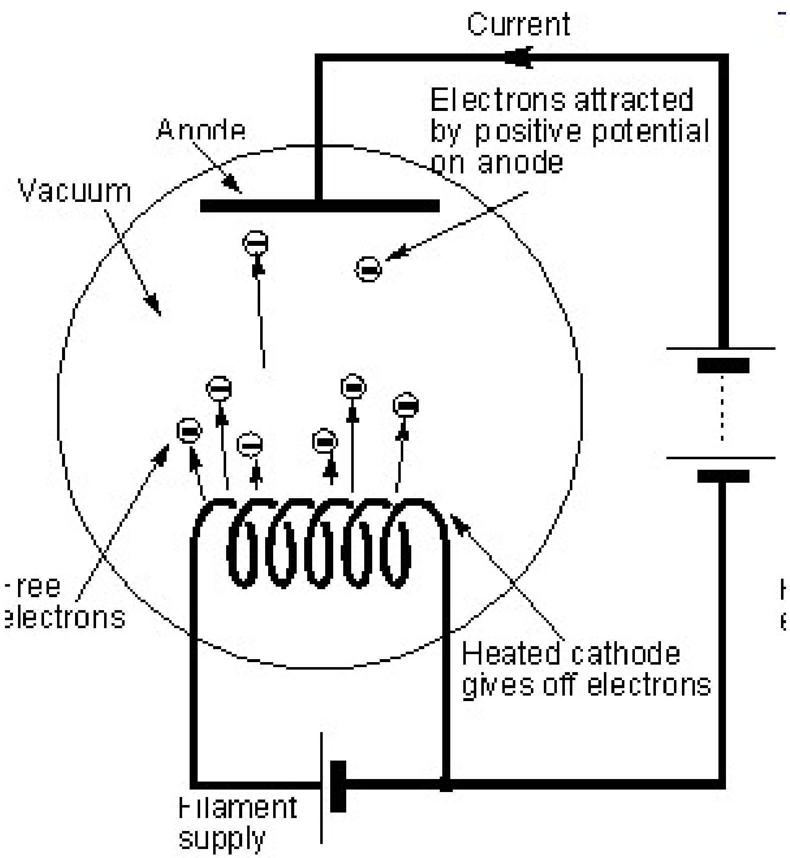
$$\vec{x} = \frac{-e\vec{E}t^2}{2m} + \vec{v}_0 t + \vec{x}_0$$

electrons in an electric field follow a parabola.

electrons in a magnetic field move in a spiral

electrons crossed electric and magnetic fields spiral along the direction perpendicular to the electric and magnetic fields

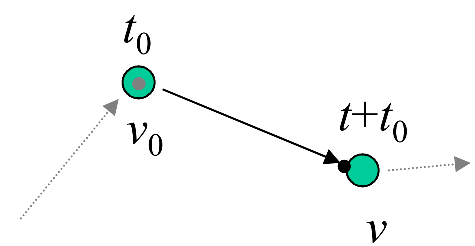
Vacuum diodes



diode

Diffusive transport

time between two collisions

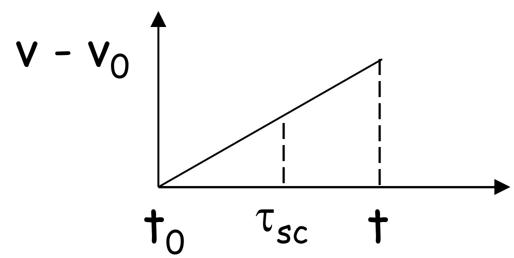


$$\vec{F} = -e\vec{E} = m^*\vec{a} = m^*\frac{d\vec{v}}{dt}$$

$$\vec{v} = \vec{v}_0 - \frac{e\vec{E}}{m^*}(t - t_0)$$

$\langle v_0 \rangle = 0$

$\langle t - t_0 \rangle = \tau_{sc}$ < average time between scattering events



$$\vec{v}_d = \frac{-e\vec{E}\tau_{sc}}{m^*} = \frac{-e\vec{E}\ell}{m^* v_F}$$

drift velocity: $\vec{v}_d = -\mu\vec{E}$

Ohm's law: $\vec{j} = -ne\vec{v}_d = ne\mu\vec{E} = \sigma\vec{E}$