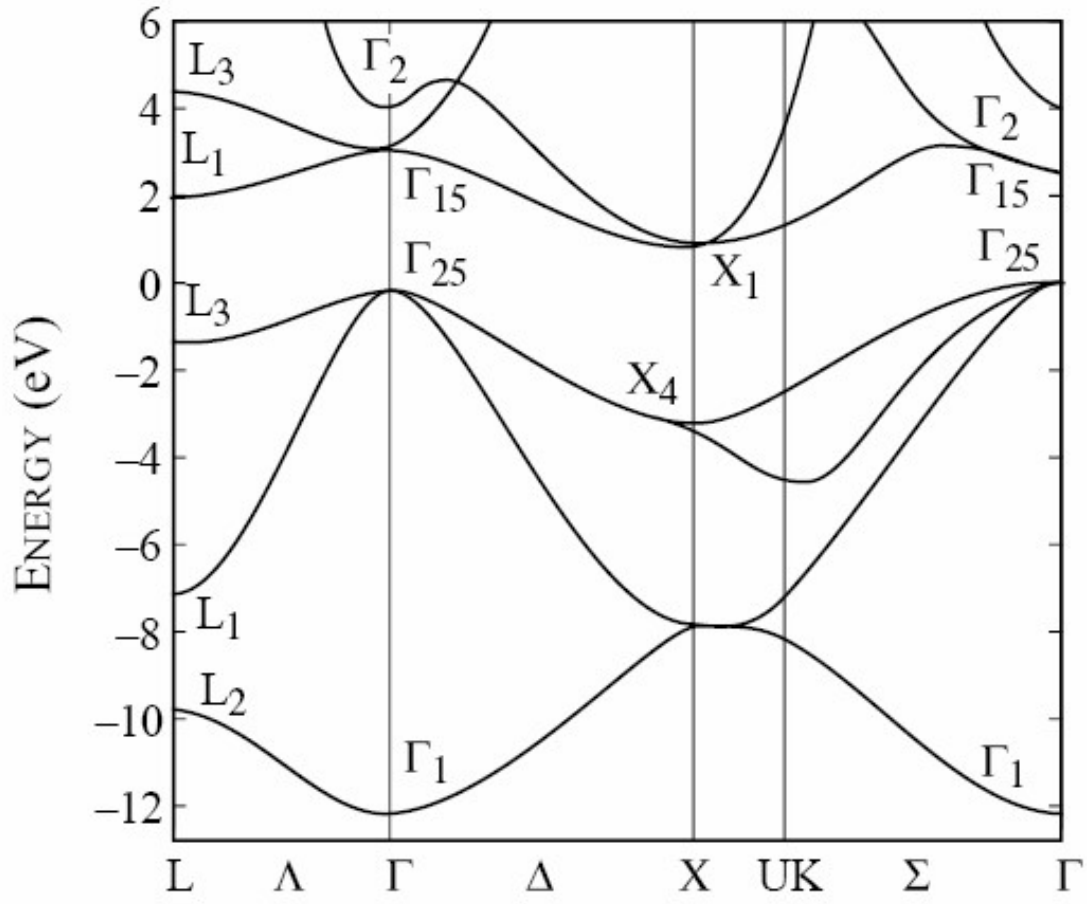
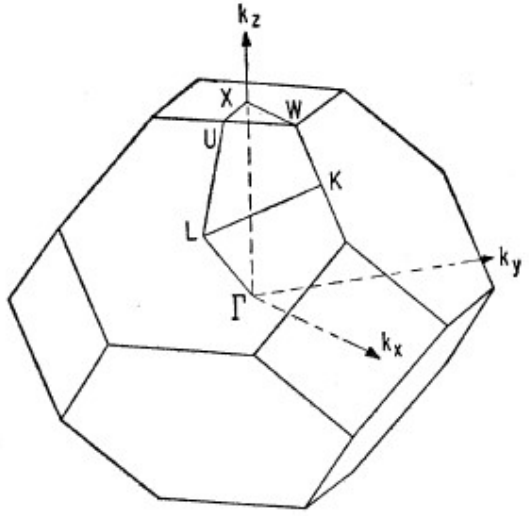
Electrons

Electron Band Theory

Calculate the dispersion relation for electrons in a crystal





silicon

2N states per Brillouin zone

A crystal $L \times L \times L$ has $N = \dfrac{L^3}{a^3}$ primitive unit cells.

The first Brillouin zone contains $N = \dfrac{\left(\dfrac{2\pi}{a}\right)^3}{\left(\dfrac{2\pi}{L}\right)^3} = \dfrac{L^3}{a^3}$ k points.

Each k state can hold 2 electrons (spin).

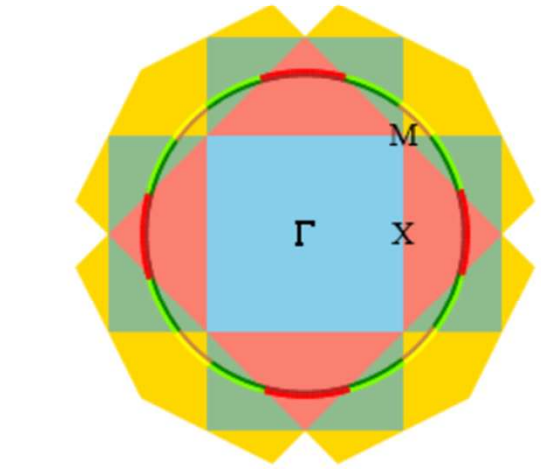
There are $2N$ electron states per Brillouin zone.

$2N$ electron states per band

Fermi surface of a two-dimensional square lattice

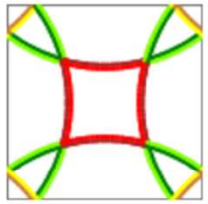
n =4.2 [-] [+] electrons/unit cell

$\frac{k_F a}{\pi}$ =1.635 $\frac{E_F}{\left[\frac{\hbar^2\pi^2}{2ma^2}\right]}$ =2.674

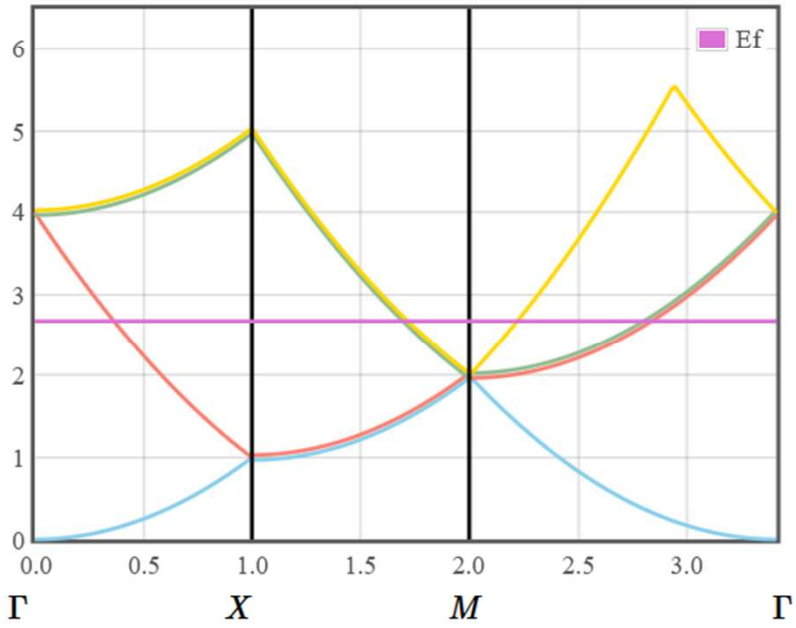


1 Bz 2 Bz 3 Bz 4 Bz

Extended Zone Scheme



Reduced Zone Scheme



http://lampx.tugraz.at/~hadley/ss2/fermisurface/2d_fermisurface/2dsquare.php

Fermi Surfaces

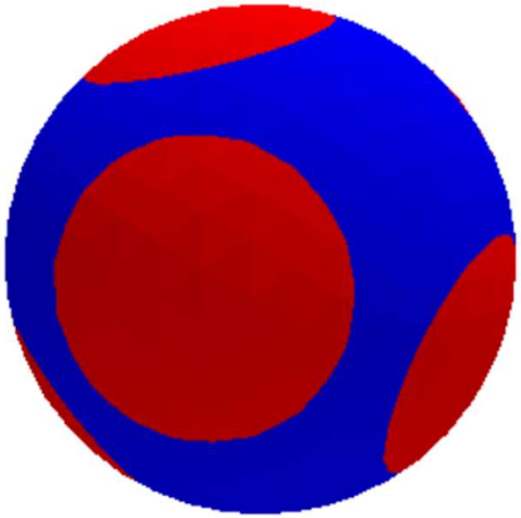
n =2 [-] [+] electrons/unit cell

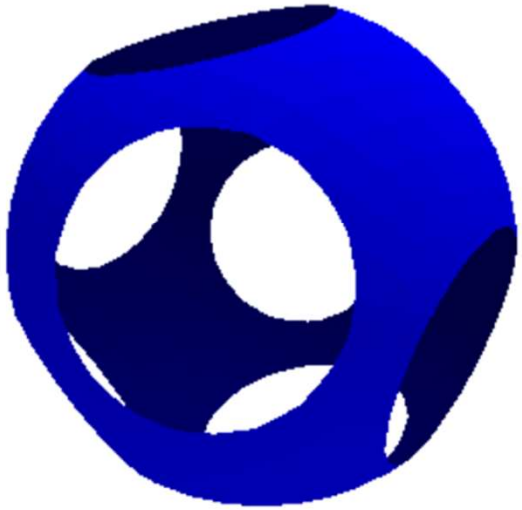
$k_F = (3\pi^2 n)^{1/3} = 3.90$

Lattice: ○ Simple Cubic ○ Body Centered Cubic ◉ Face Centered Cubic ○ Hexagonal Close Pack $\frac{c}{a} = \sqrt{\frac{8}{3}}$

[Show 1st Brillouin zone] [Stop Rotation]

Brillouinzone	1	2	3	4
Outside Color				
Inside Color				
Show	☑	☐	☑	☑





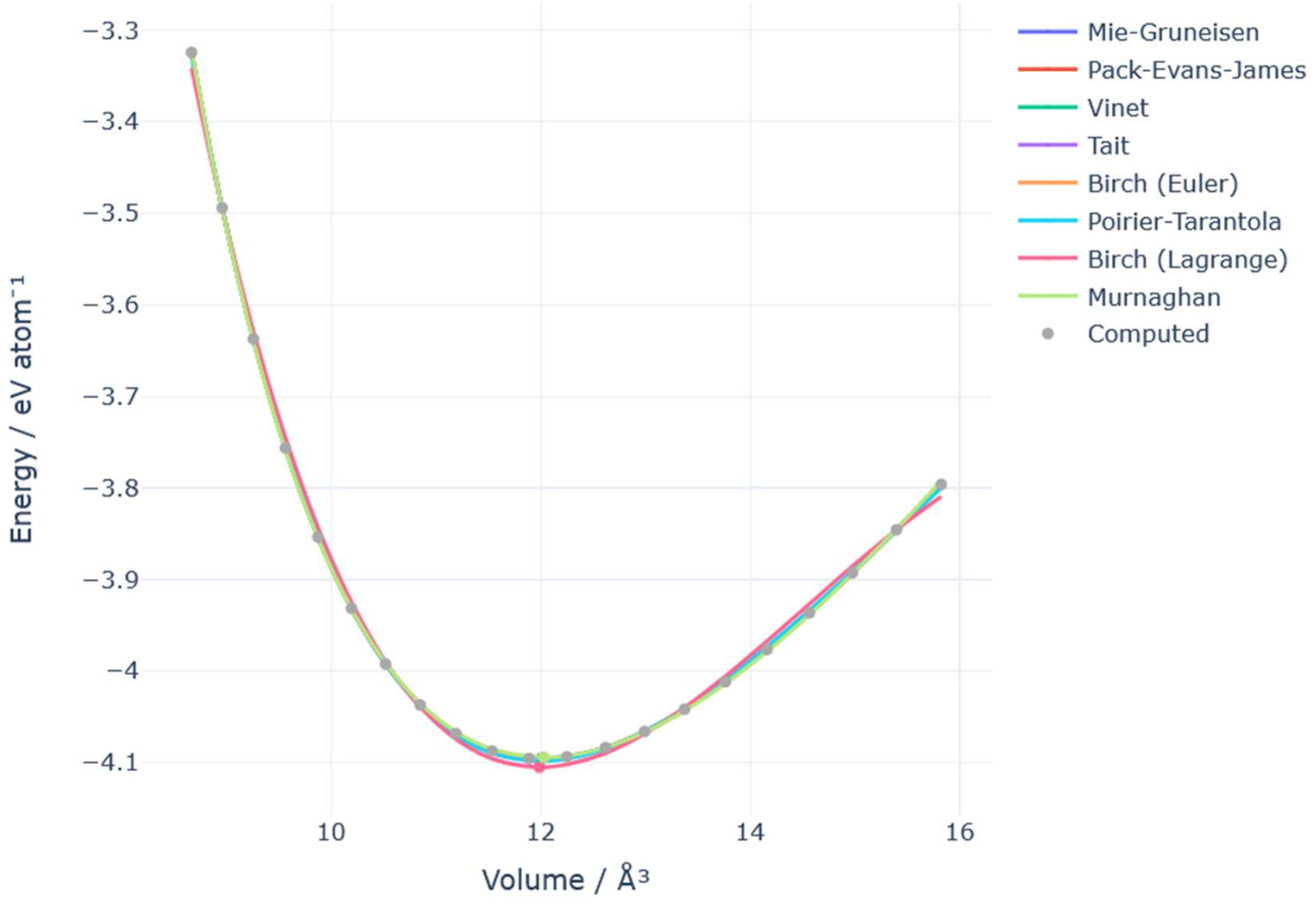
http://lampx.tugraz.at/~hadley/ss2/fermisurface/3d_fermisurface/index.html

Band structure calculations

Knowing how the atoms are arranged, calculate the electron states

Density Functional Theory (DFT)
Plane wave method
Tight binding

Band structure calculations



Tight binding

Tight binding does not include electron-electron interactions

$$H_{MO} = \frac{-\hbar^2}{2m_e}\nabla^2 - \sum_A \frac{Z_A e^2}{4\pi\varepsilon_0 \left|\vec{r} - \vec{r}_A\right|}$$

$$\psi_k = \frac{1}{\sqrt{N}} \sum_{l,m,n} \exp\left(i\left(l\vec{k}\cdot\vec{a}_1 + m\vec{k}\cdot\vec{a}_2 + n\vec{k}\cdot\vec{a}_3\right)\right)\psi_{\text{unit\_cell}}\left(\vec{r} - l\vec{a}_1 - m\vec{a}_2 - n\vec{a}_3\right)$$

$$\psi_{\text{unit\_cell}}\left(\vec{r}\right) = \sum_i c_i \phi_i\left(\vec{r} - \vec{r}_i\right)$$

Atomic wave functions

This is the tight-binding wave function.

$$H_{MO}\psi_k = E_k\psi_k$$

Tight binding: 1-D chain

$$\psi_k(x) = \frac{1}{\sqrt{N}} \sum_n e^{inka} \phi(x - na)$$

Substitute the tight-binding wave function into the time independent Schrödinger equation.

$$H_{MO}\psi_k = E_k\psi_k$$

Multiply from the left by the atomic orbitals.

$$\langle \phi(x) | \hat{H} | \psi_k(x) \rangle = E \langle \phi(x) | \psi_k(x) \rangle$$

$$\langle \phi(x) | \hat{H} | \phi(x-a) \rangle e^{-ika} + \langle \phi(x) | \hat{H} | \phi(x) \rangle + \langle \phi(x) | \hat{H} | \phi(x+a) \rangle e^{ika} + \text{small terms}$$

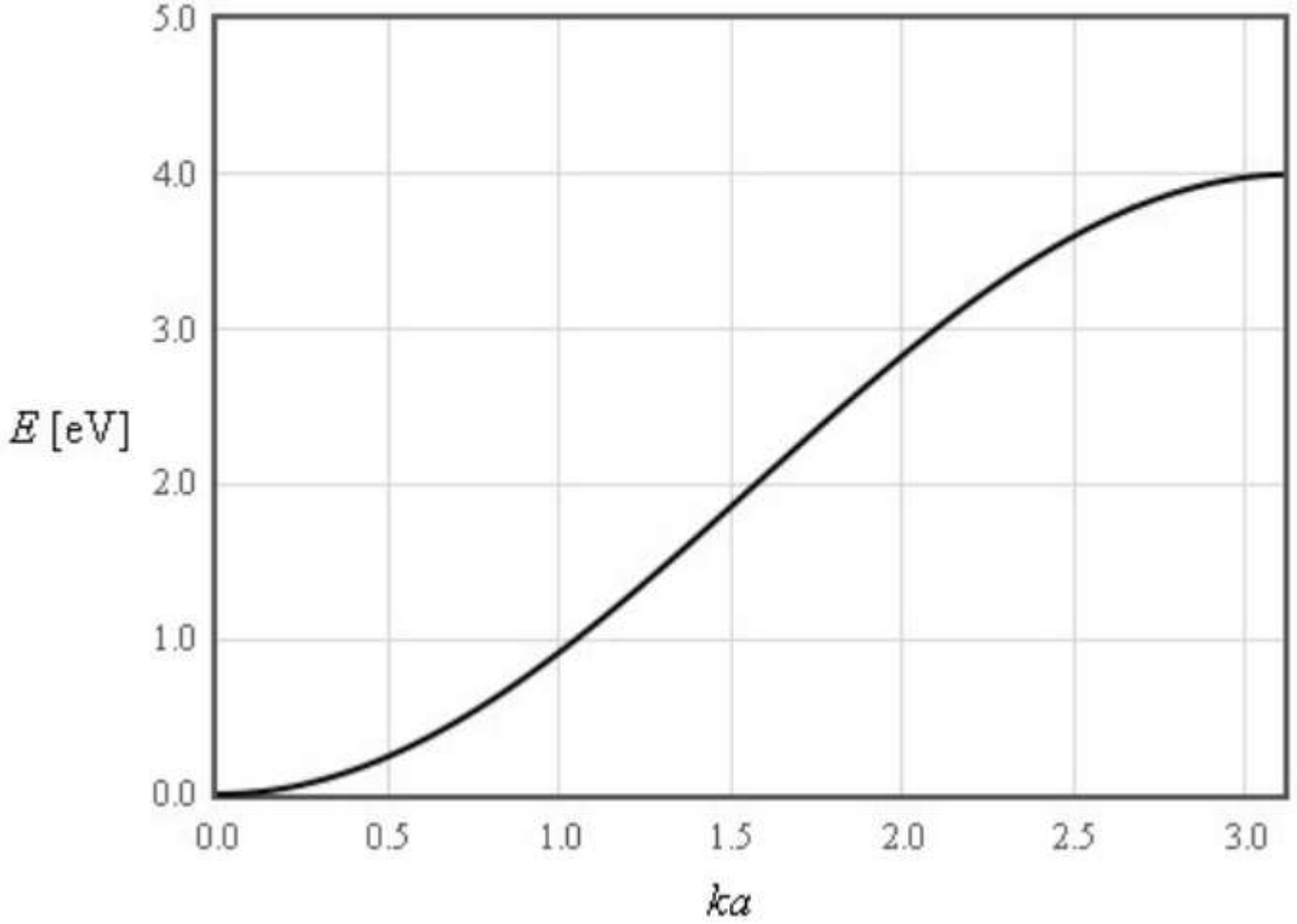
$$= E + \text{small terms}.$$

$$\epsilon = \langle \phi(x) | \hat{H} | \phi(x) \rangle \text{ and } t = -\langle \phi(x) | \hat{H} | \phi(x-a) \rangle$$

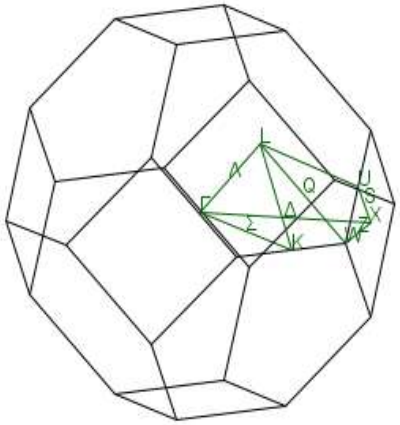
$$E = \epsilon - t\left(e^{-ika} + e^{-ika}\right) = \epsilon - 2t\cos(ka).$$

Tight binding: 1-D chain

$$E = \epsilon - 2t\cos(ka).$$

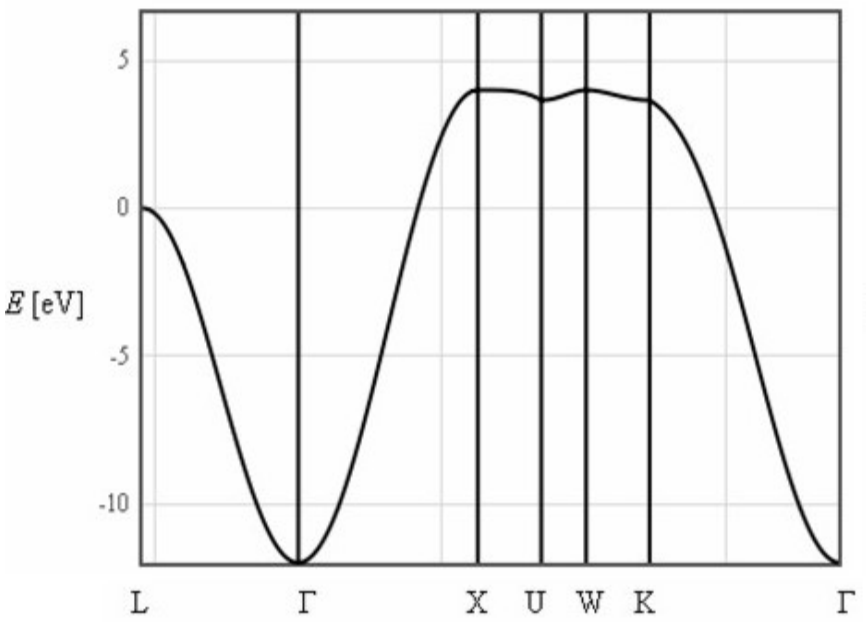


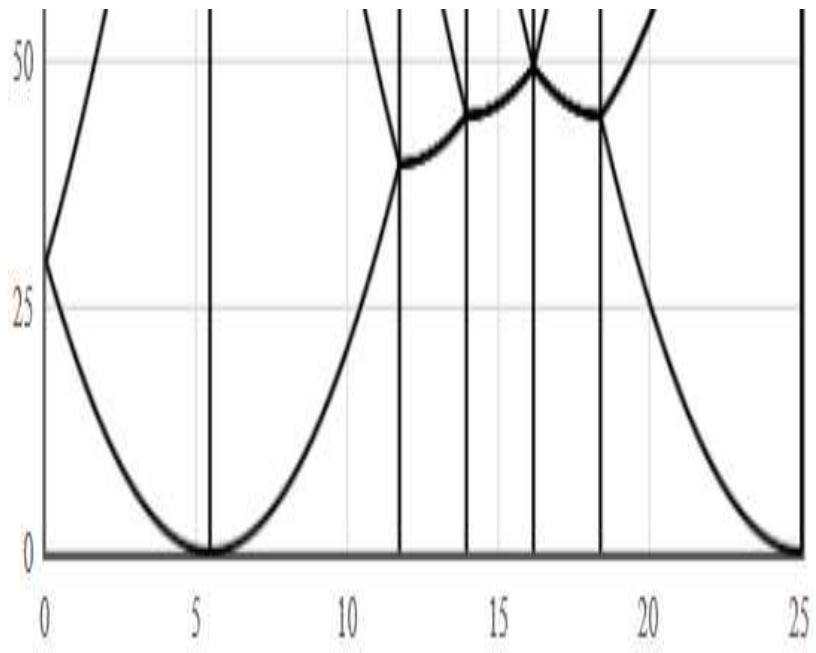
Tight binding, fcc



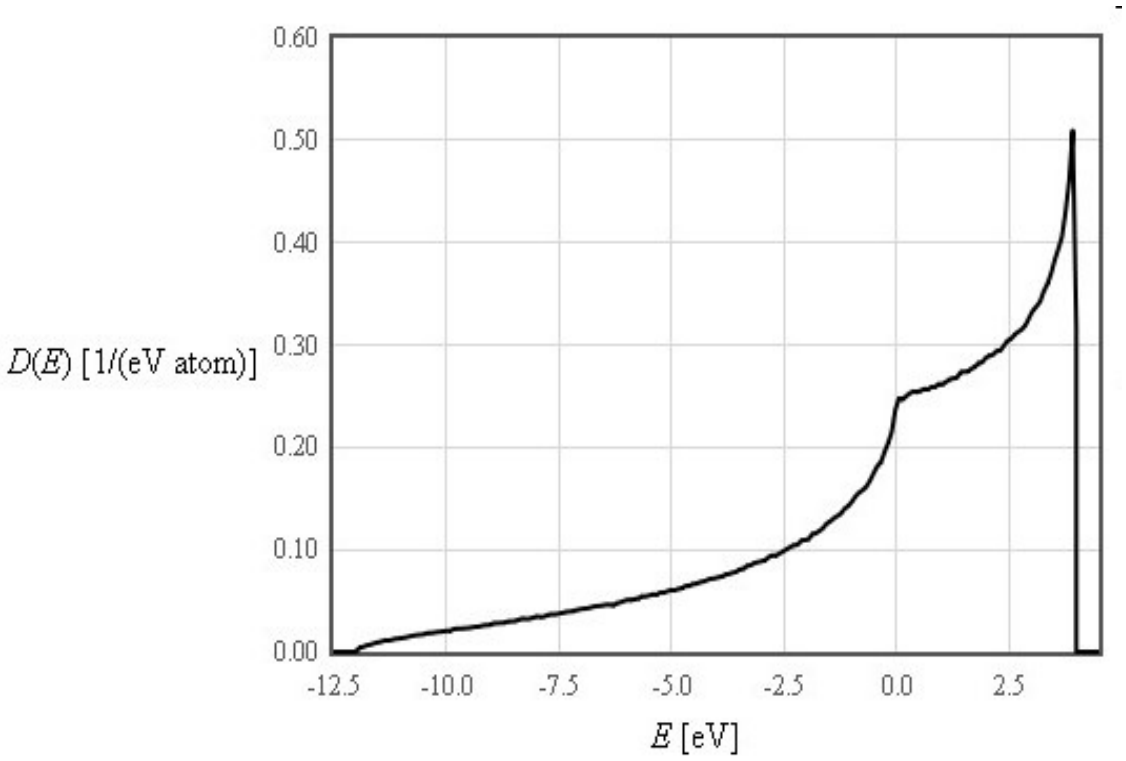
$$E = \varepsilon - t\sum_{lmn} e^{i\vec{k}\cdot\vec{\rho}_{lmn}}$$

$$E = \varepsilon - 4t\left(\cos\left(\frac{k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right) + \cos\left(\frac{k_x a}{2}\right)\cos\left(\frac{k_z a}{2}\right) + \cos\left(\frac{k_y a}{2}\right)\cos\left(\frac{k_z a}{2}\right)\right)$$





Density of states (fcc)

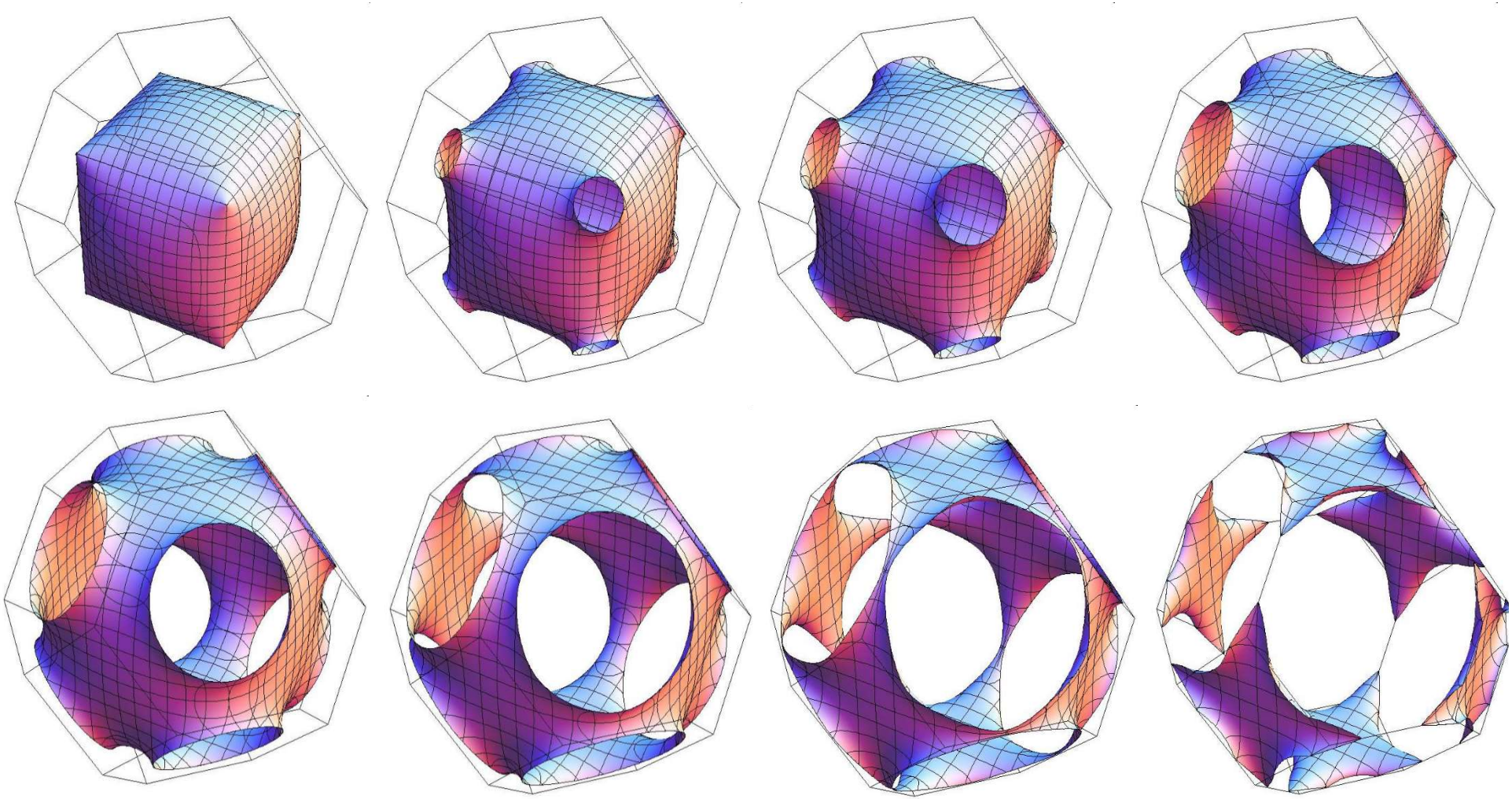


Calculate the energy for every allowed k in the Brillouin zone

$$E = \varepsilon - 4t\left(\cos\left(\frac{k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right) + \cos\left(\frac{k_x a}{2}\right)\cos\left(\frac{k_z a}{2}\right) + \cos\left(\frac{k_y a}{2}\right)\cos\left(\frac{k_z a}{2}\right)\right)$$

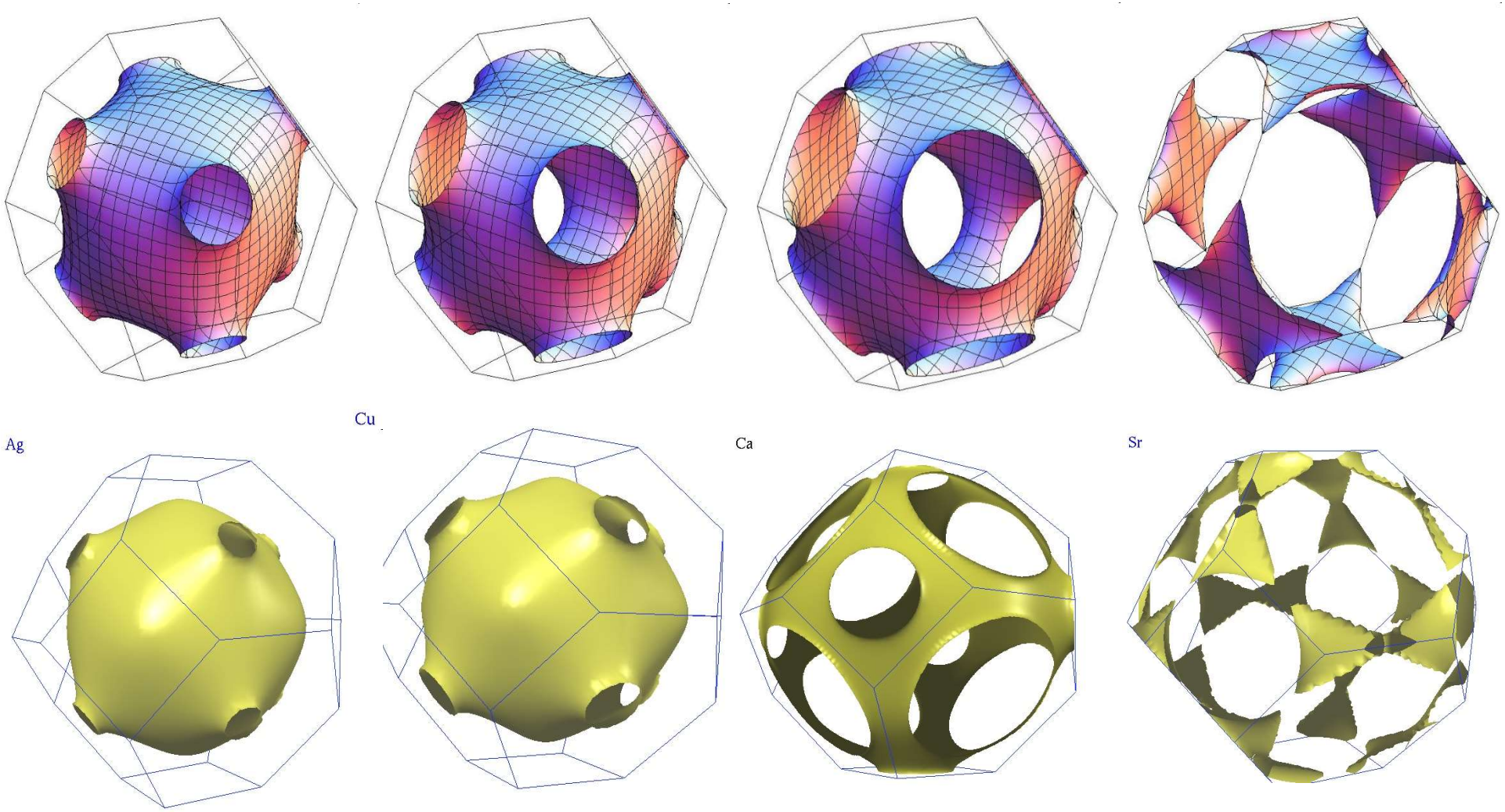
http://lamp.tu-graz.ac.at/~hadley/ss1/bands/tbtable/tbtable.html

Tight binding, fcc

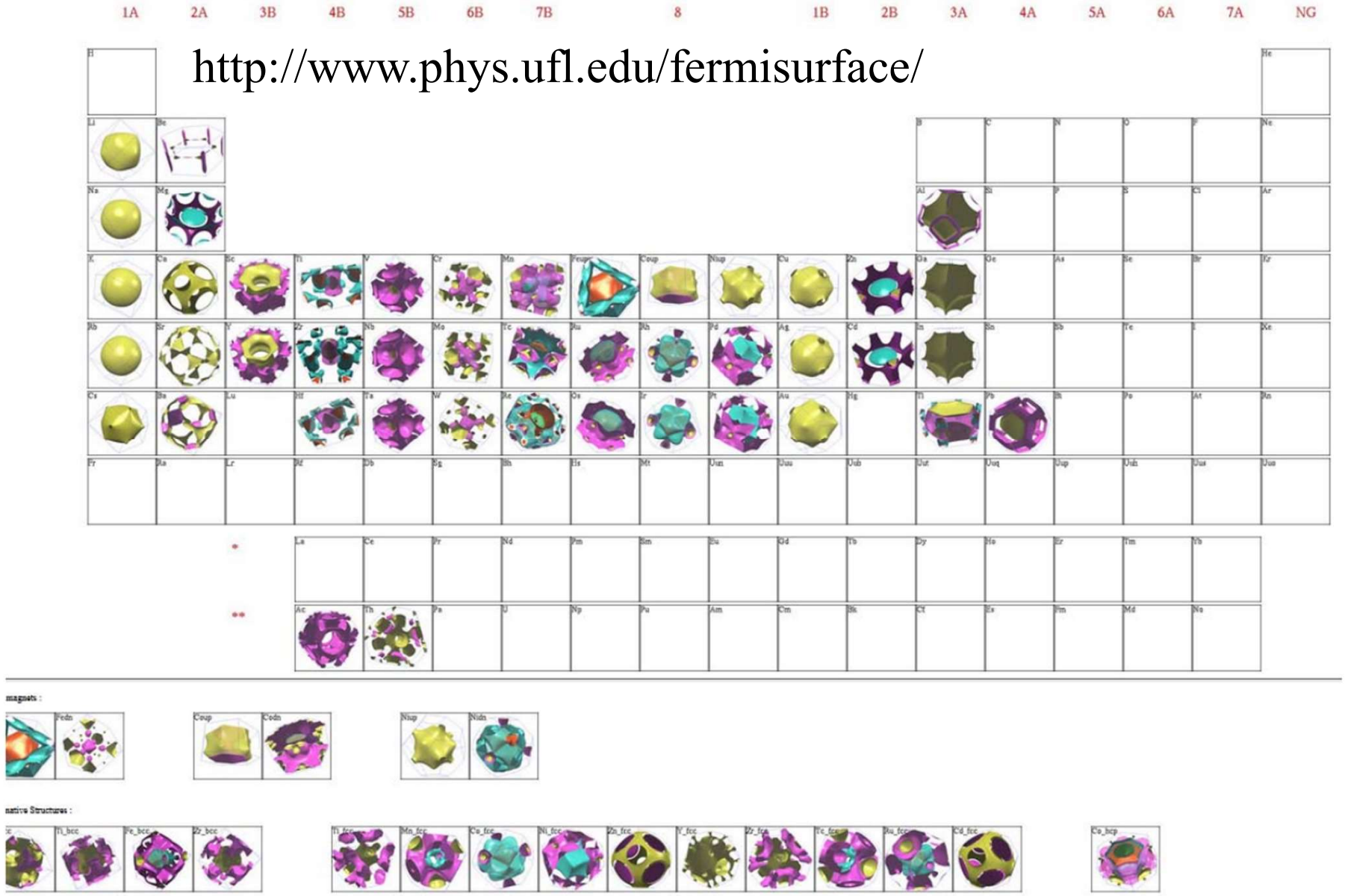


Christian Gruber, 2008

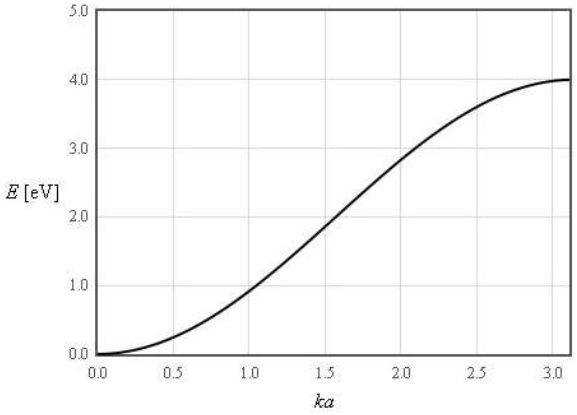
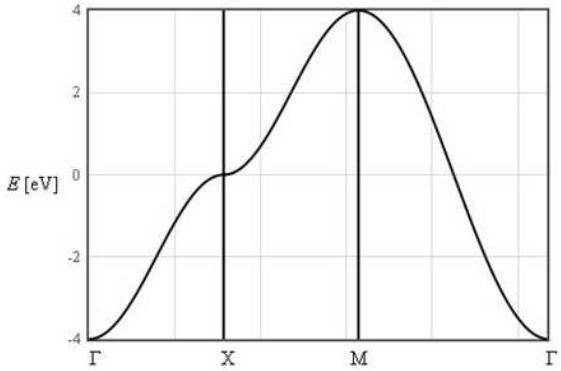
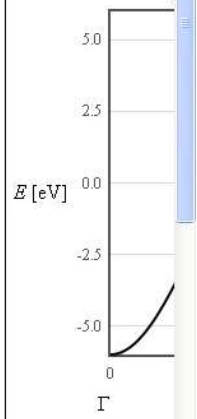
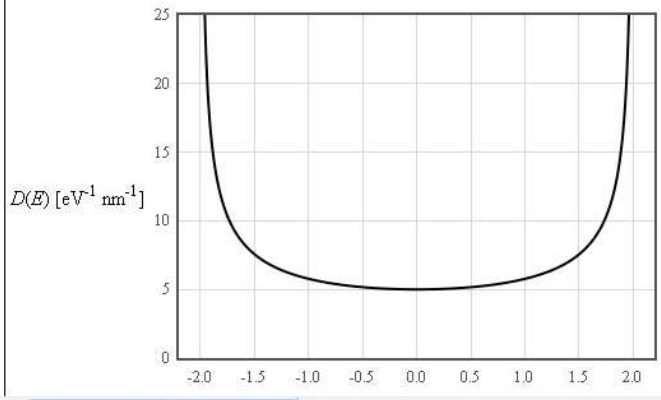
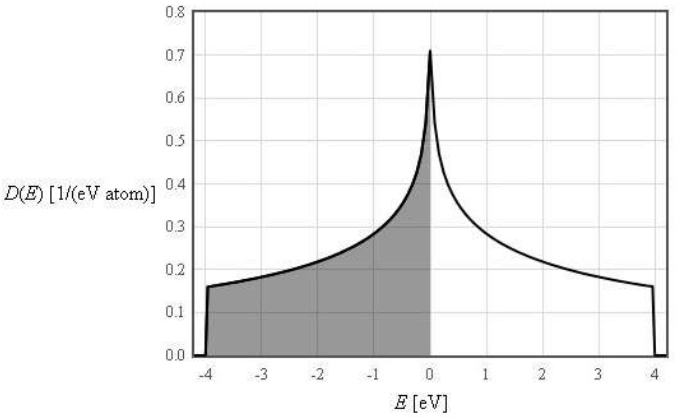
Tight binding, fcc



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


1A
2A
3B
4B
5B
6B
7B
8
1B
2B
3A
4A
5A
6A
7A
NG
http://www.phys.ufl.edu/fermisurface/
magnets :
native Structures :

http://lamp.tu-graz.ac.at/~hadley/ss1/bands/tbtable/tbtable.html

	Linear Chain	2-D square lattice	
relation	$E = \varepsilon - 2t\cos(k_x a)$  Calculate E(k)	$E = \varepsilon - 2t\left(\cos(k_x a) + \cos(k_y a)\right)$  Calculate E(k)	$E = \varepsilon - 2t$ 
of states	$D(k) = \frac{2}{\pi}$	$D(k) = \frac{k}{\pi}$ m^{-1}	
of states	$D(E) = \frac{1}{at\sqrt{1-\left(\frac{\varepsilon - E}{2t}\right)^2}}$ $\mathrm{J}^{-1}\mathrm{m}^{-1}$ 		D(E) [1/(eV

[Simple Periodic Table with the electronic band structure of each element]

H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag							
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au							

[png images, less than about 20 kb](Start 2/2, 2006)(
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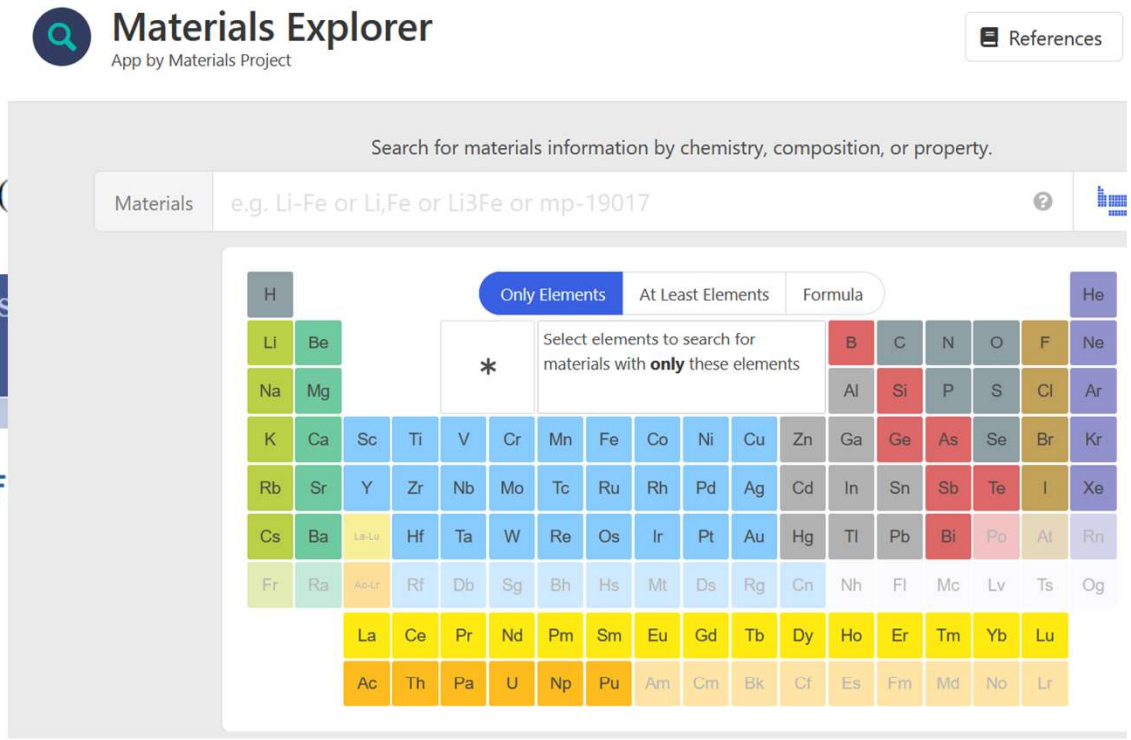
Characteristics and Properties

Semiconductors n,k database InGaAsP Levels

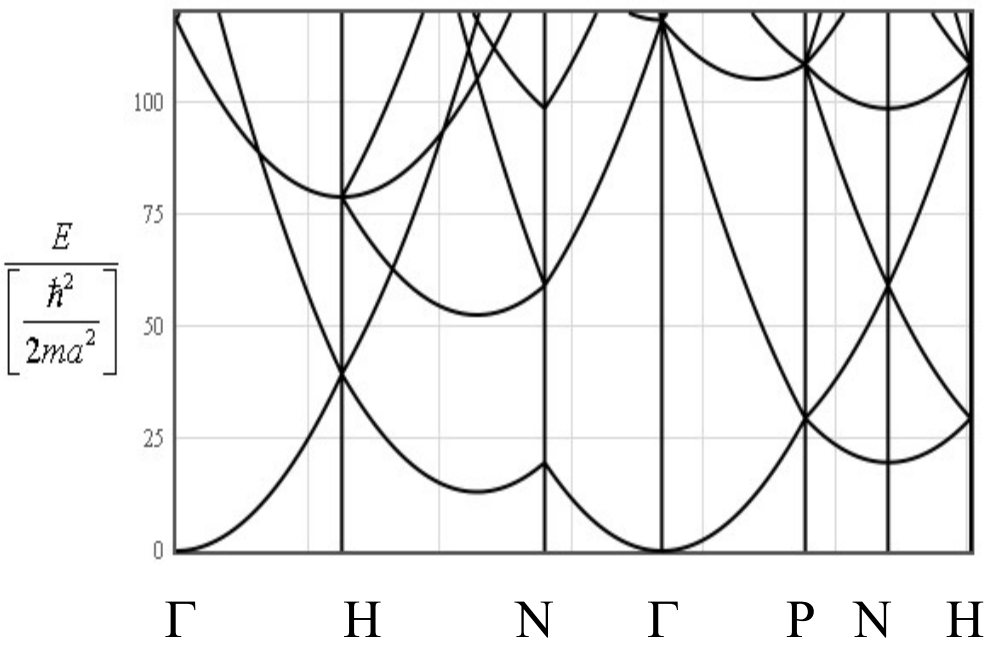
NSM Archive - Physical Properties of

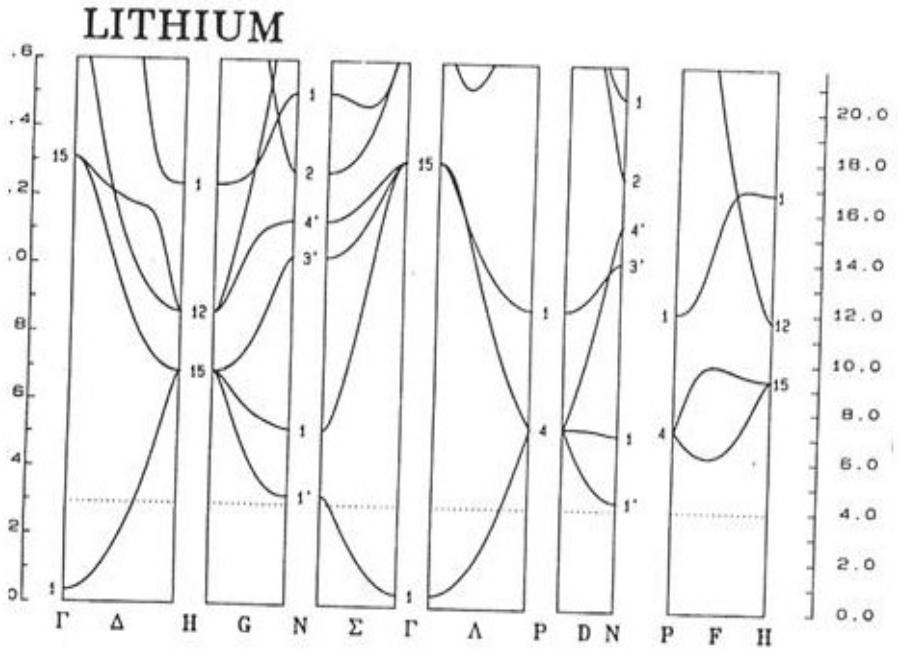
Si	- Silicon
GaP	- Gallium Phosphide
InAs	- Indium Arsenide
GaSb	- Gallium Antimonide
InP	- Indium Phosphide
$Al_xGa_{1-x}As$	- Aluminium Gallium Arsenide
AlN	- Aluminium Nitride
BN	- Boron Nitride

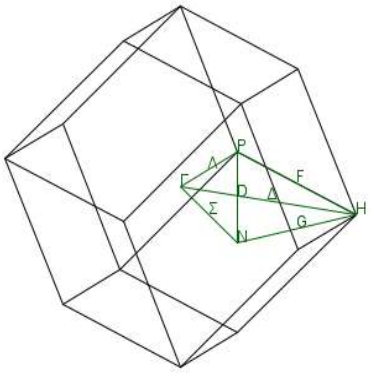


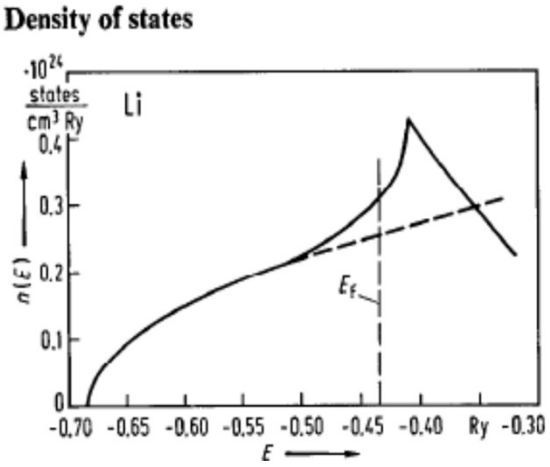
$GaAs_{1-x}Sb_x$	- Gallium Arsenide Antimonide
InN	- Indium Nitride
GaN	- Gallium Nitride

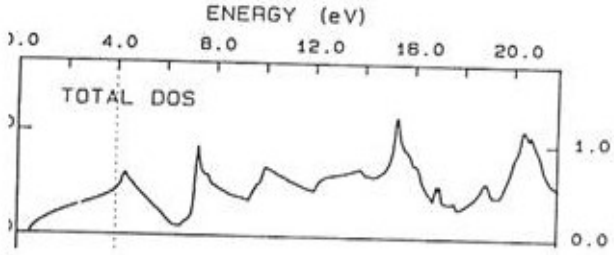
Lithium bcc


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


LITHIUM
Γ Δ H G N Σ Γ Λ P D N P F H


P
Γ
Δ
D
Σ
N
G
H


Density of states
$\cdot 10^{24}$ states / cm³ Ry
Li
0.4
0.3
0.2
0.1
0
n(E)
E_F
-0.70 -0.65 -0.60 -0.55 -0.50 -0.45 -0.40 Ry -0.30
E


ENERGY (eV)
4.0
8.0
12.0
16.0
20.0
TOTAL DOS
1.0
0.0

Sodium

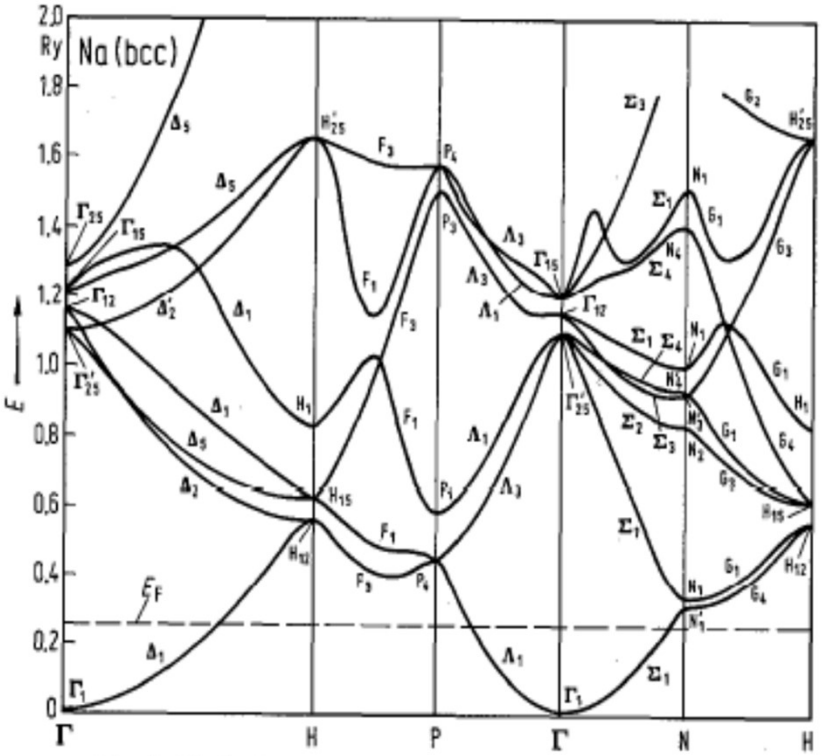
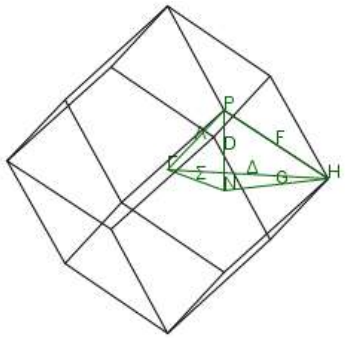
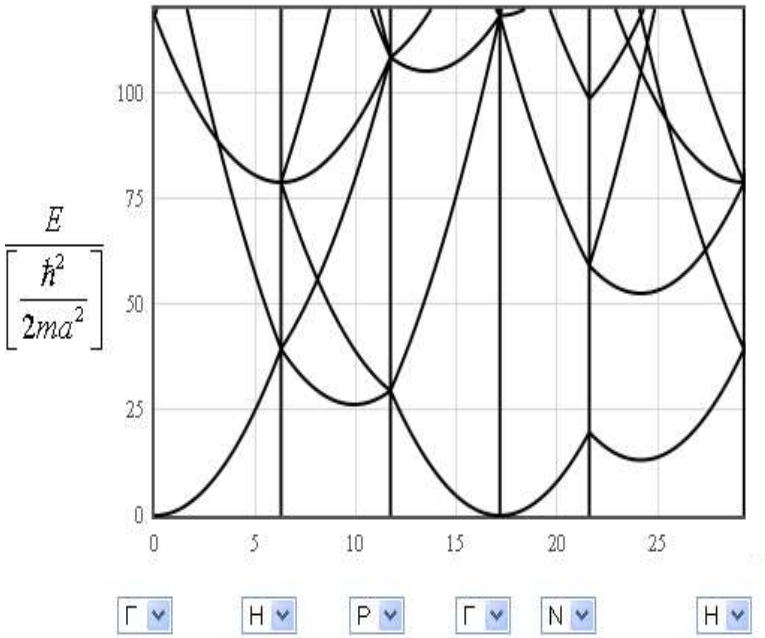
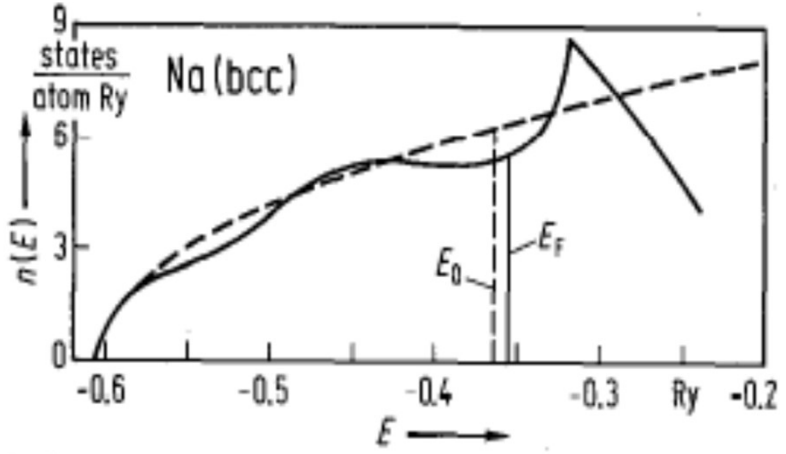
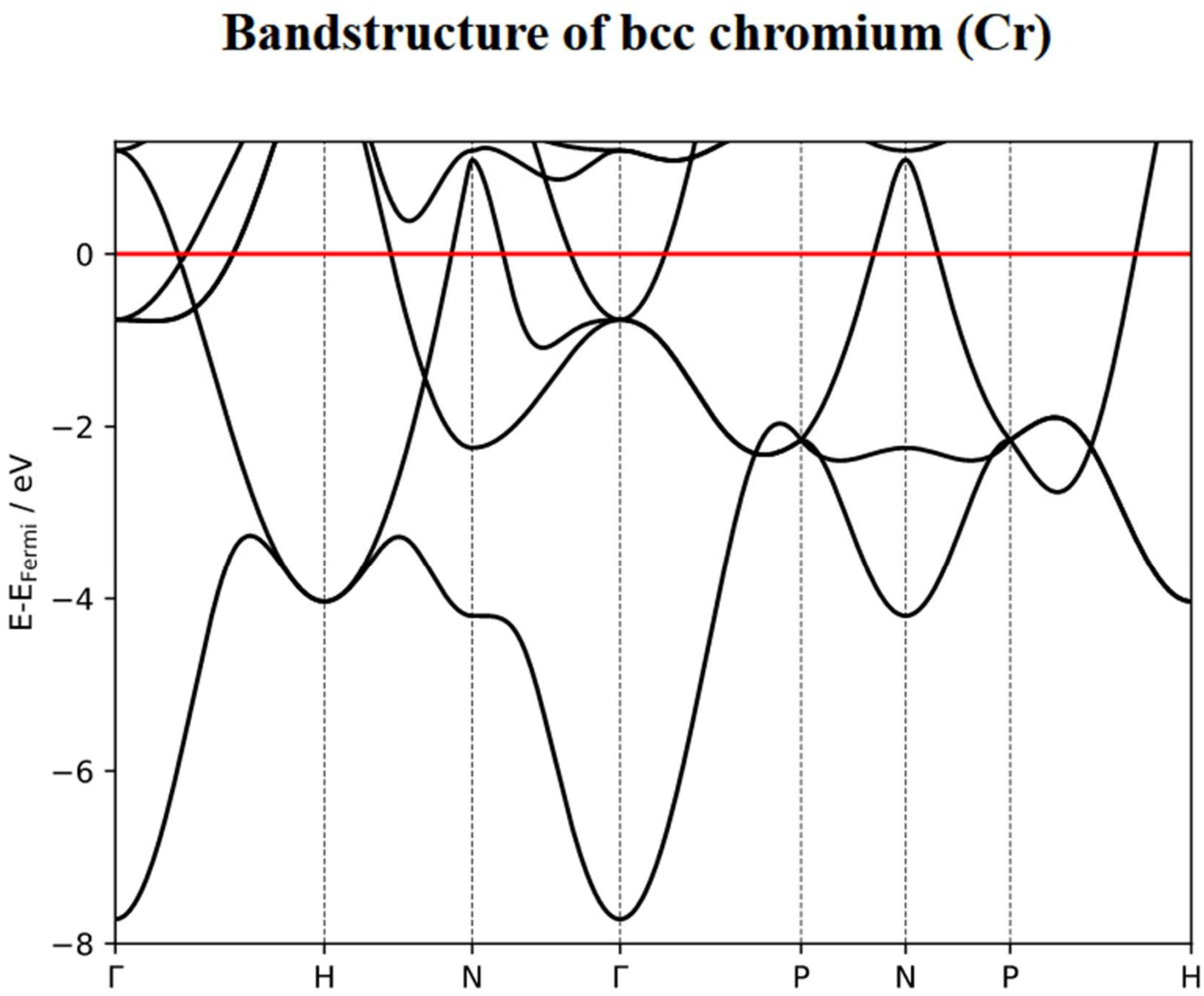


Fig. 6. Na (bcc). Energy bands calculated using the APW method by Gupta (quoted in [73Haq]).



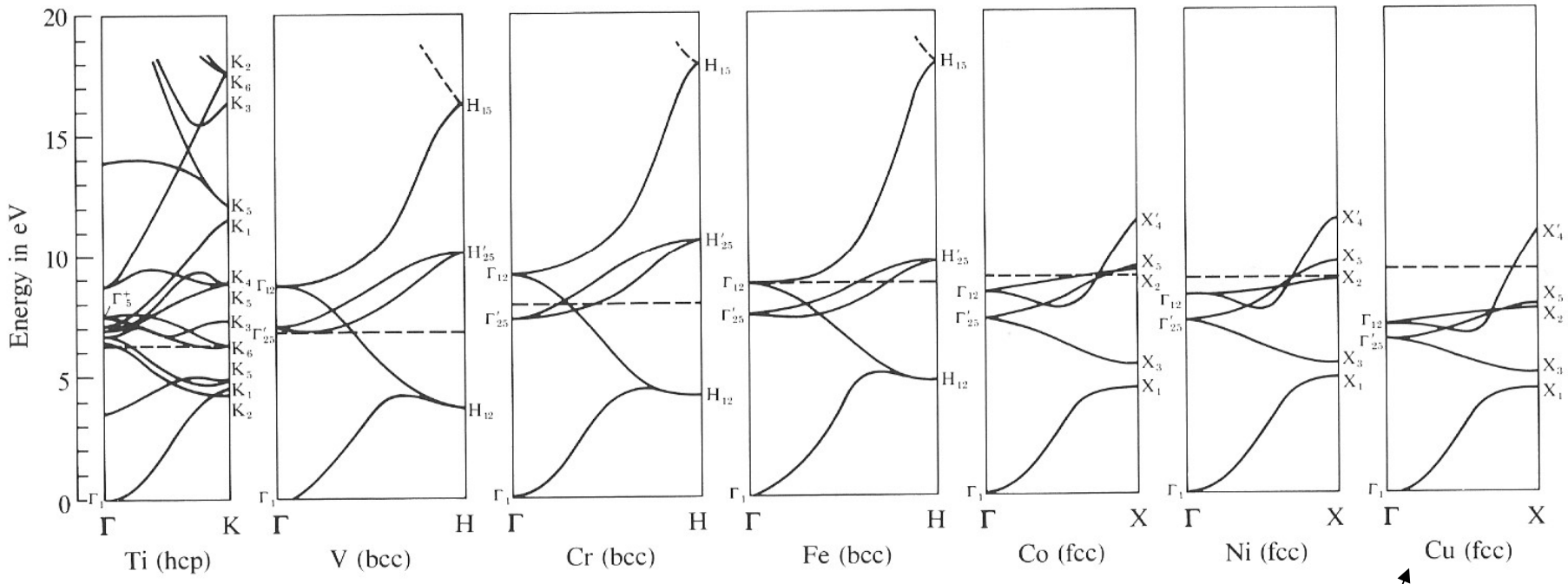


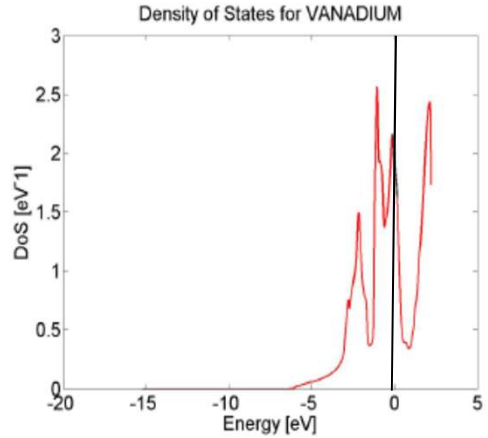


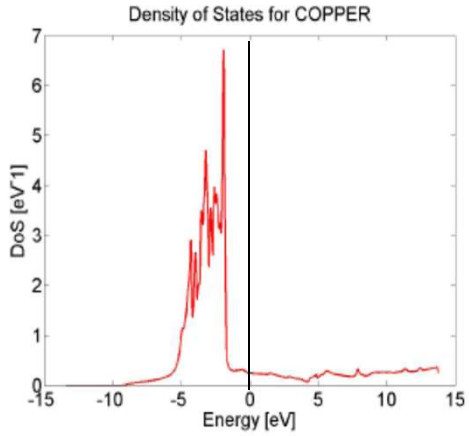


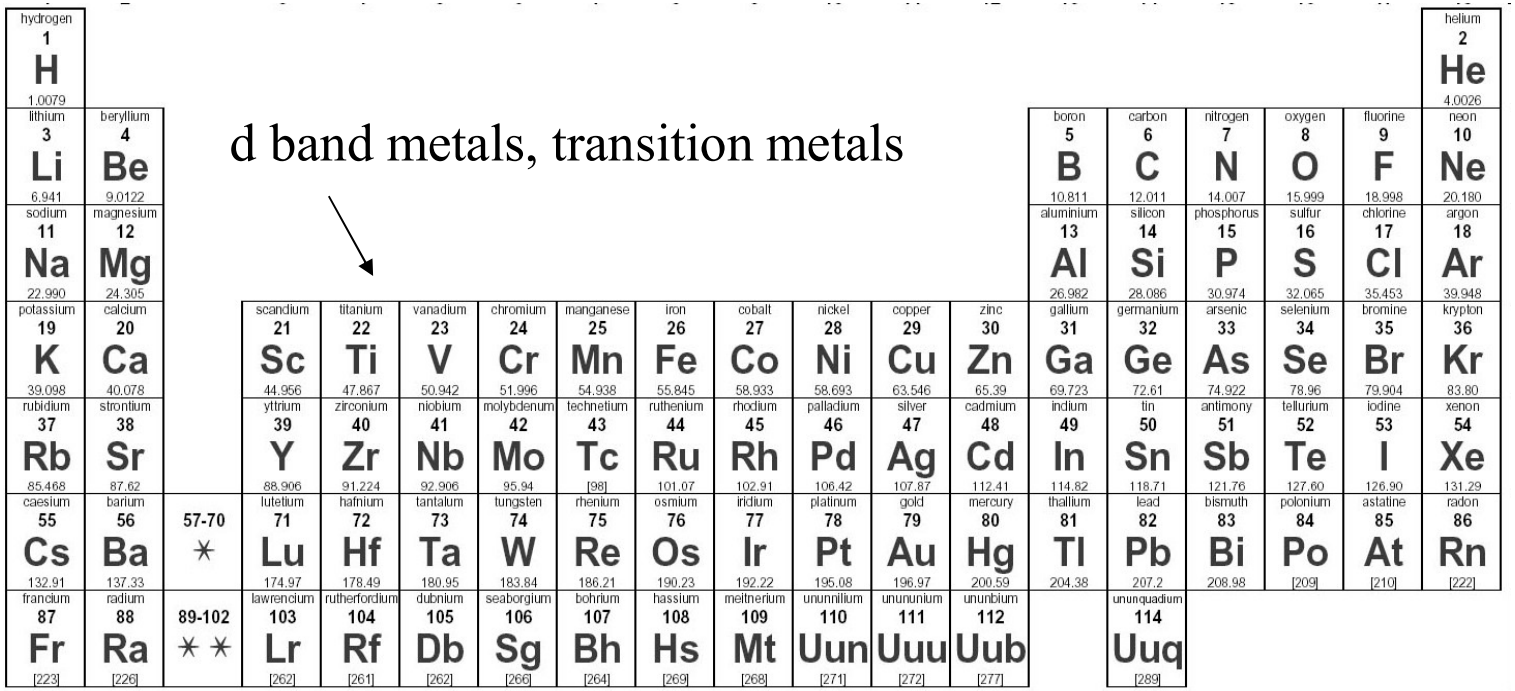
http://lampx.tugraz.at/~hadley/ss1/bands/bandstructures/Cr/Cr_Bandstructure.html

Transition metals

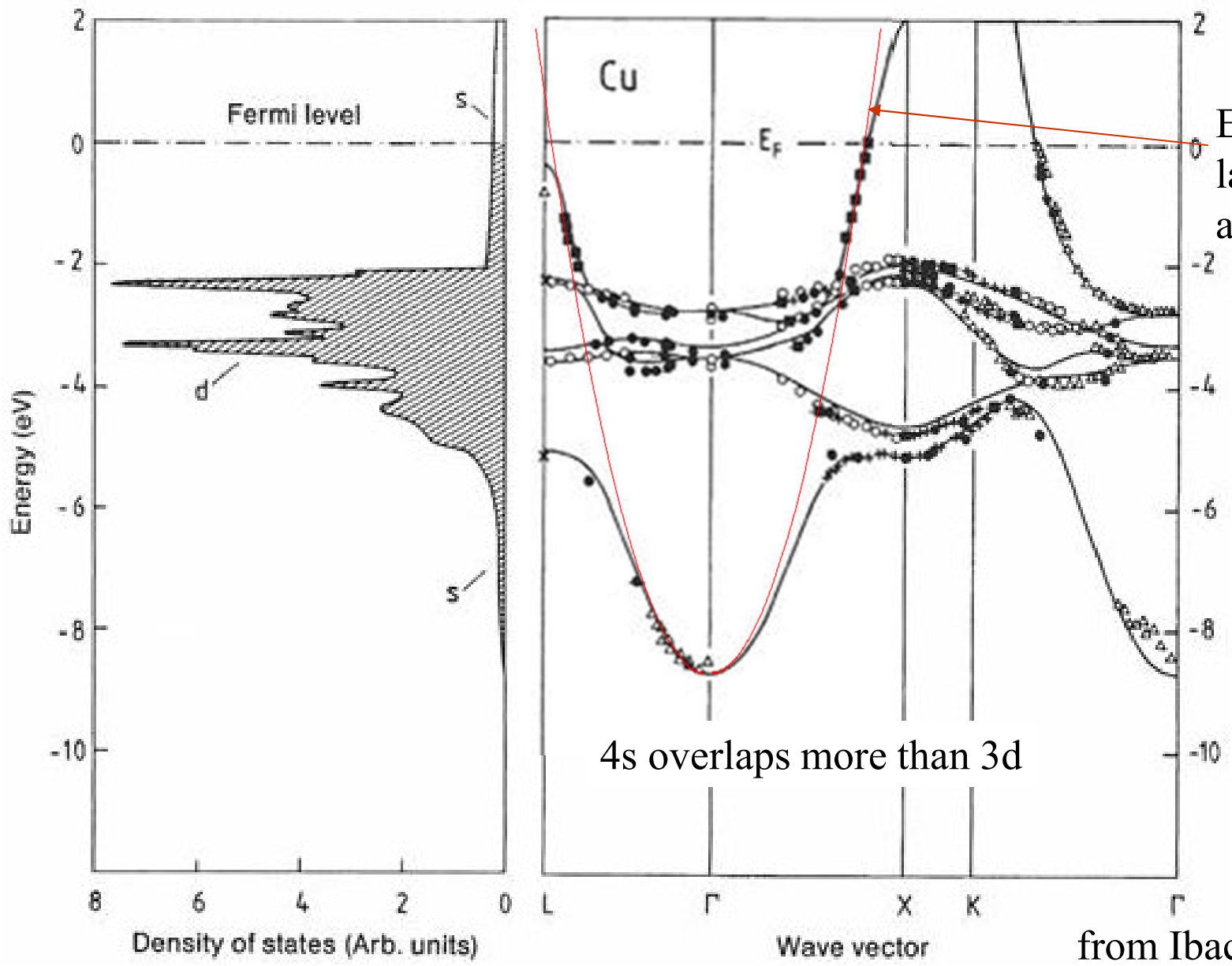







d band metals, transition metals
hydrogen 1 H 1.0079
helium 2 He 4.0026
lithium 3 Li 6.941
beryllium 4 Be 9.0122
boron 5 B 10.811
carbon 6 C 12.011
nitrogen 7 N 14.007
oxygen 8 O 15.999
fluorine 9 F 18.998
neon 10 Ne 20.180
sodium 11 Na 22.990
magnesium 12 Mg 24.305
aluminium 13 Al 26.982
silicon 14 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]
*Lanthanide series
**Actinide 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
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

Copper dispersion relation and density of states



from Ibach & Lueth

Silver

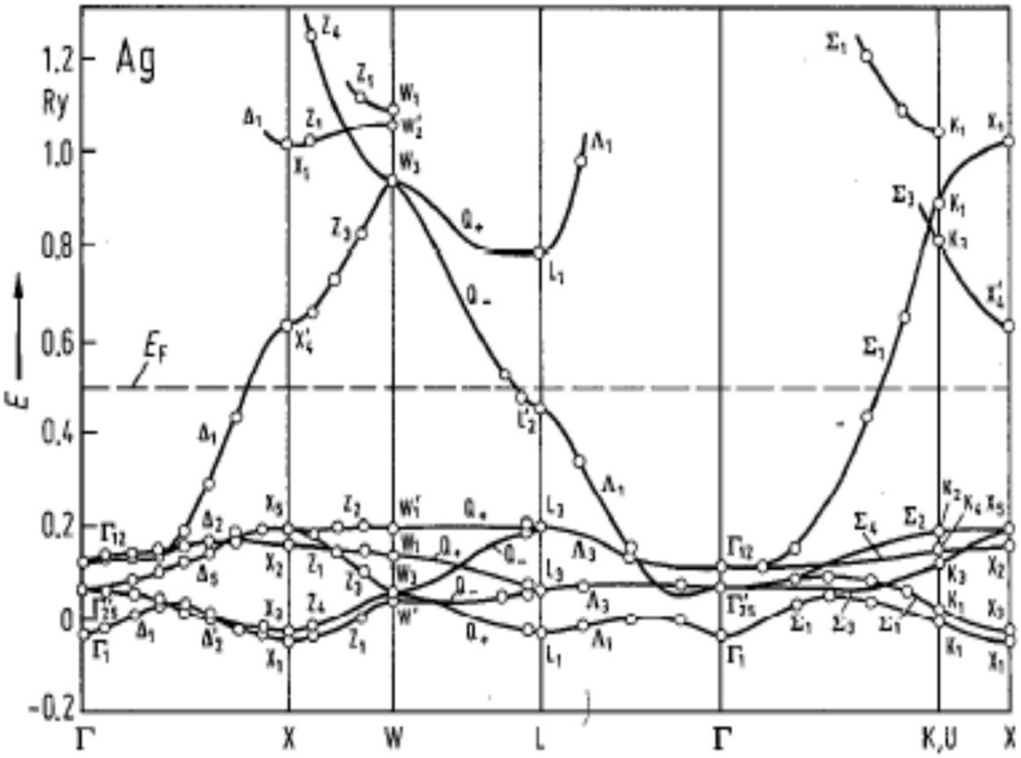


Fig. 3. Ag. Energy bands calculated using the APW method [69Chr].

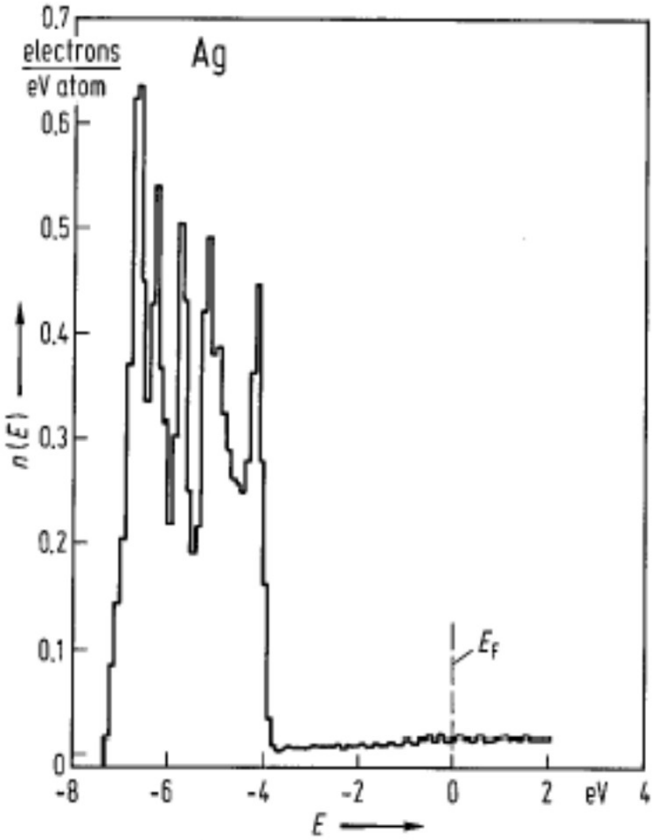
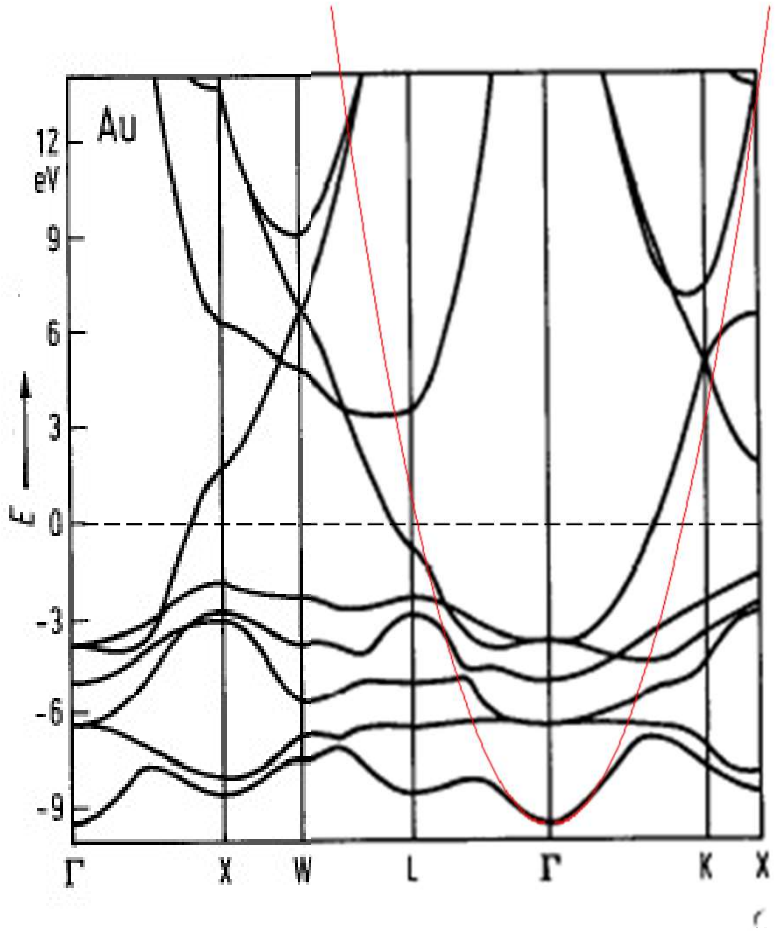


Fig. 15. Ag. Density of states calculated from the energy bands in Fig. 10. Ag [75Fon].

Gold



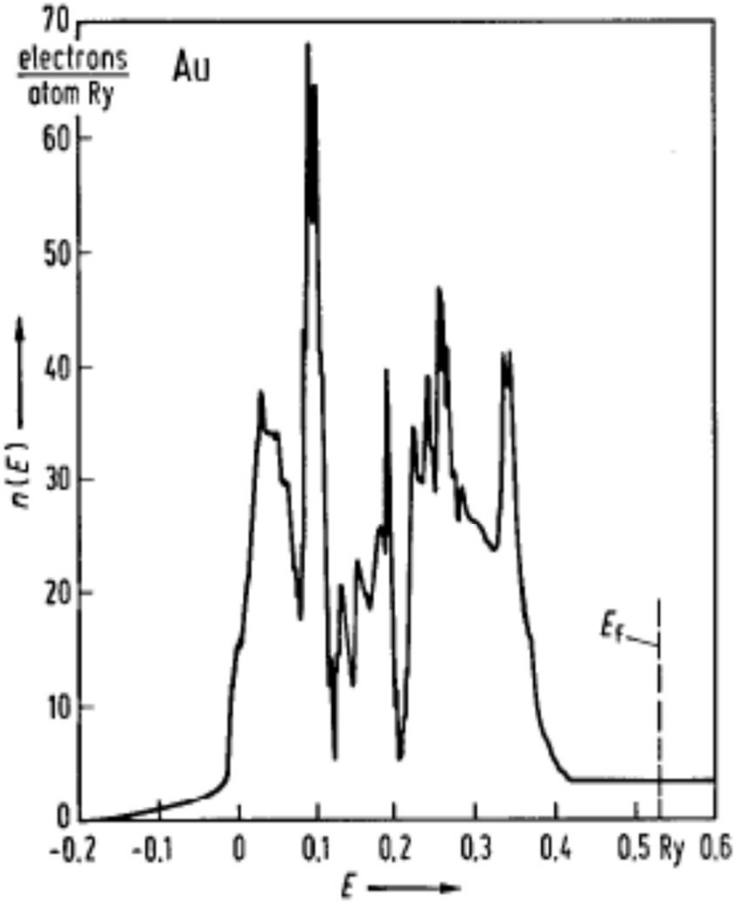
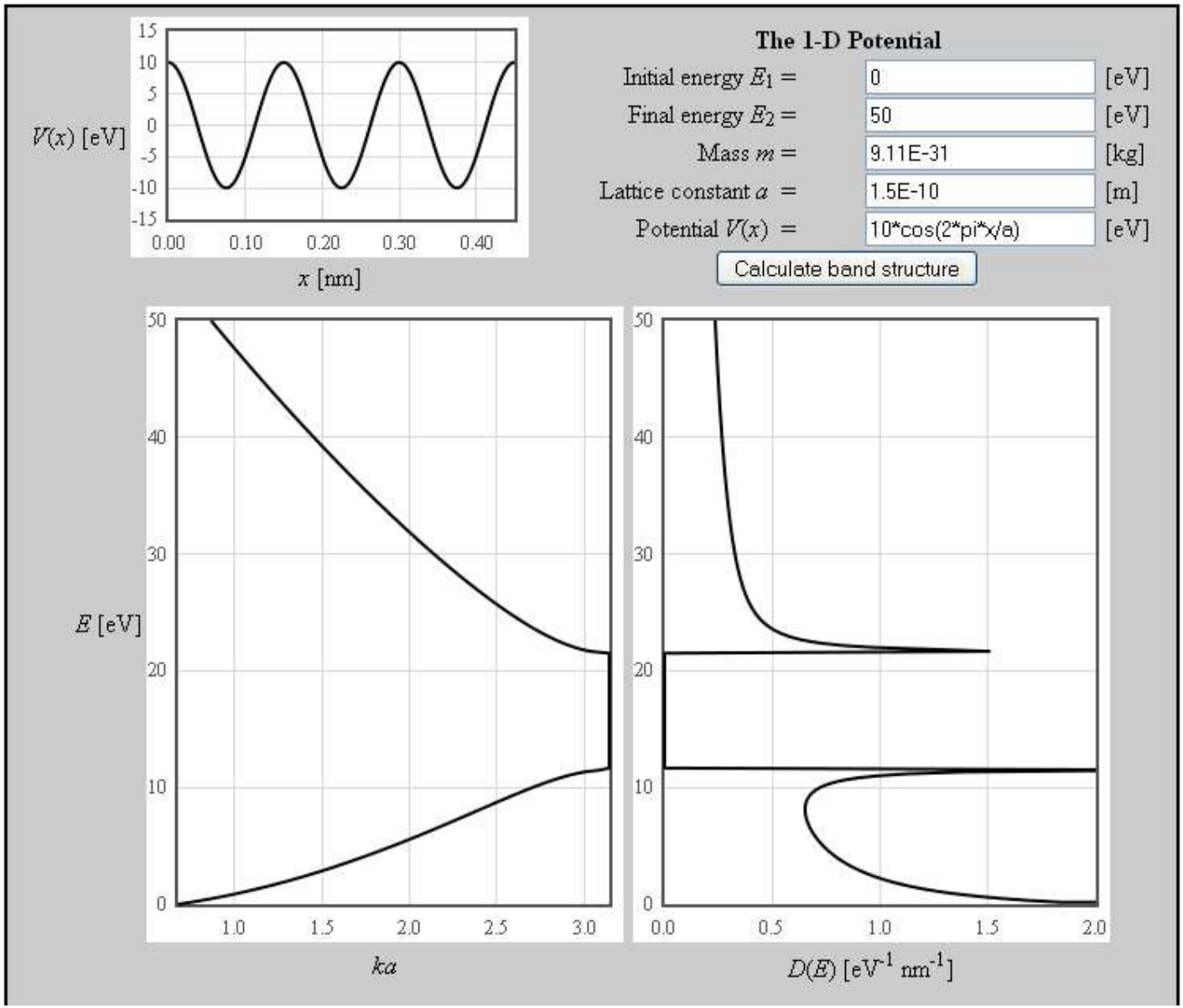


Fig. 9. Au. Density of states calculated from the energy bands in Fig. 4b. Au [71Chr2].

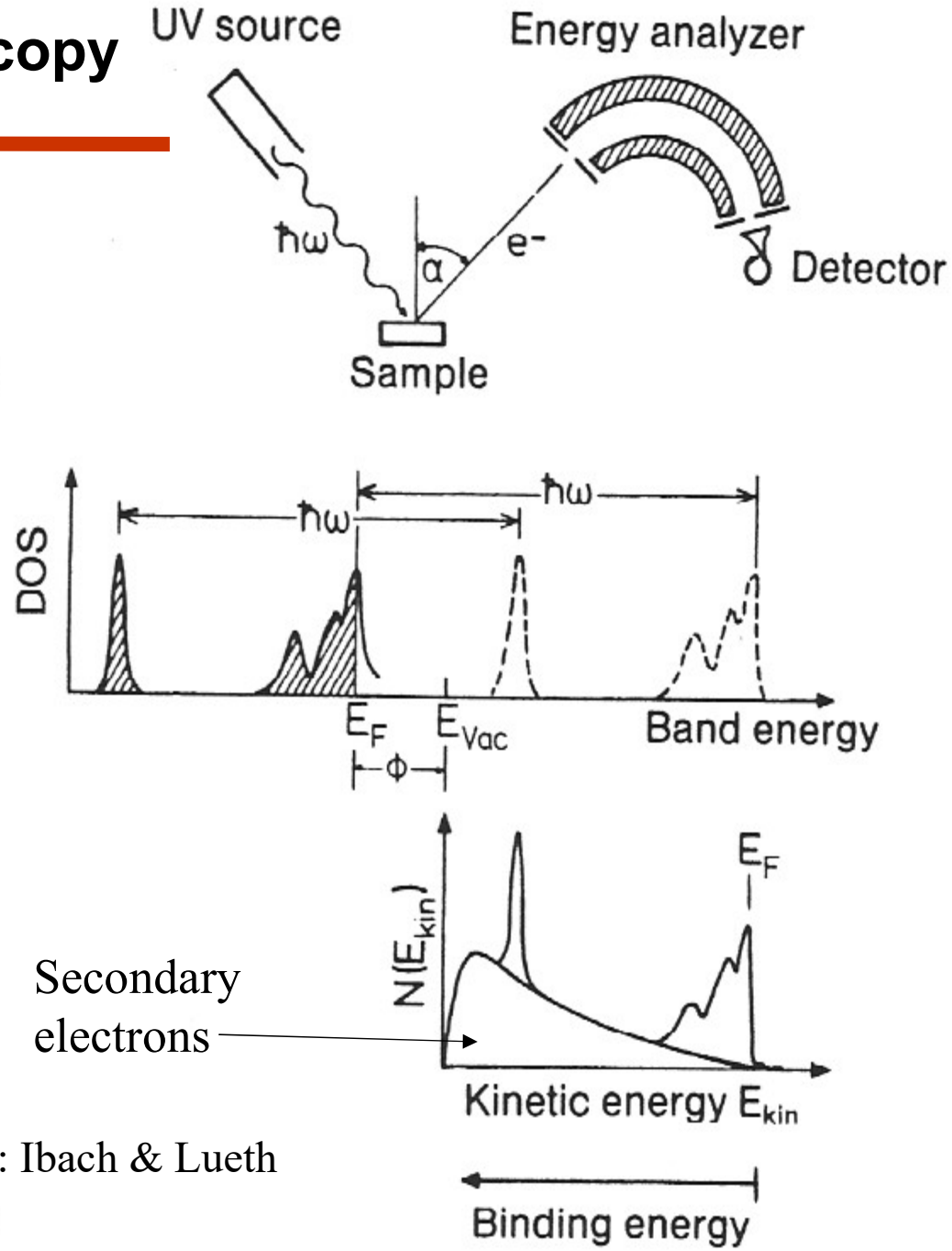
Band structure in 1-D



Photoemission spectroscopy

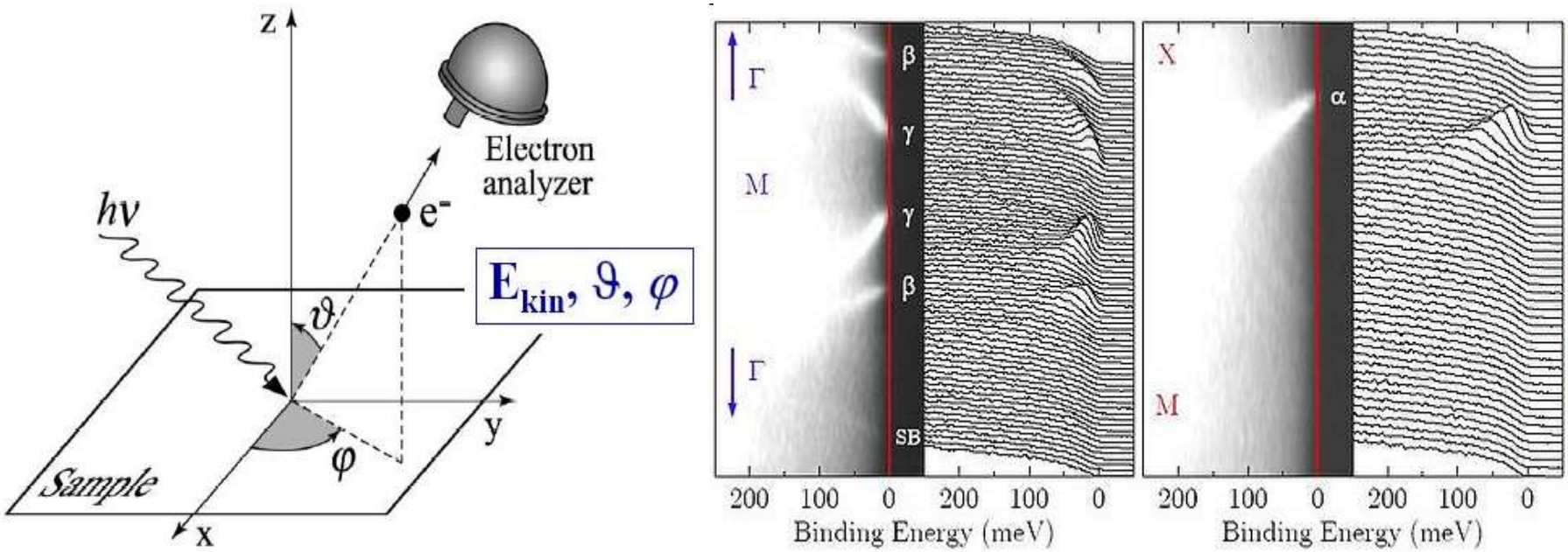
UPS - Ultraviolet photoemission spectroscopy

Measure the density of states with photoemission spectroscopy



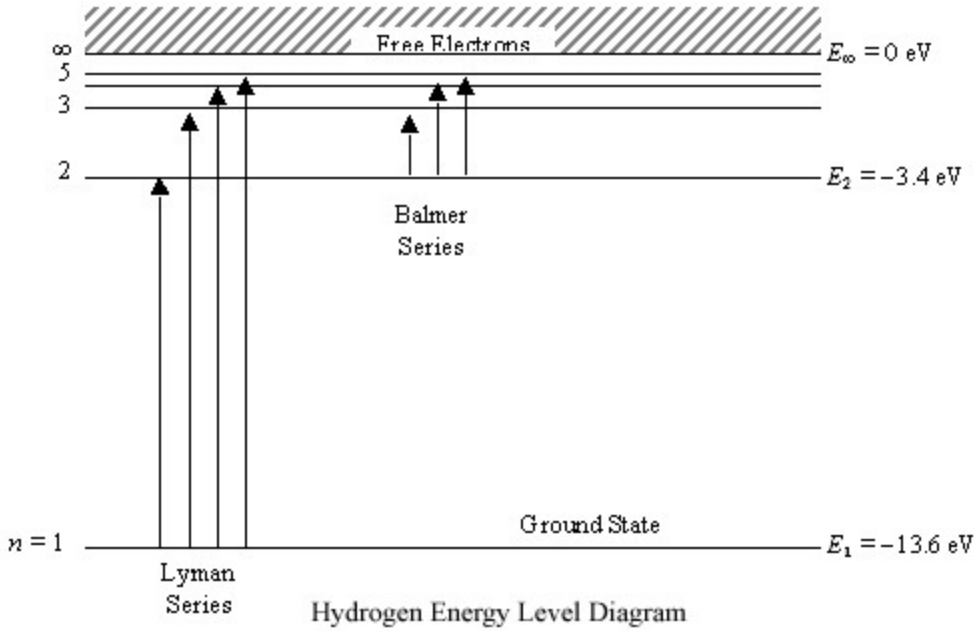
From: Ibach & Lueth

Angle resolved photoemission spectroscopy (ARPES)



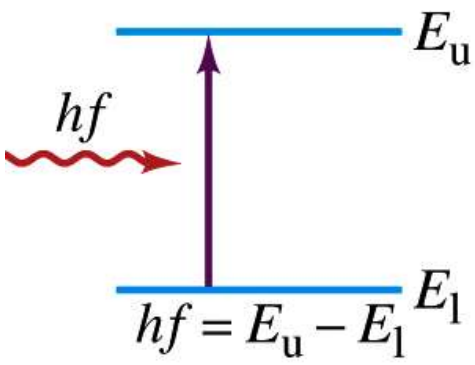
Measure the dispersion relation with angle resolved photoemission

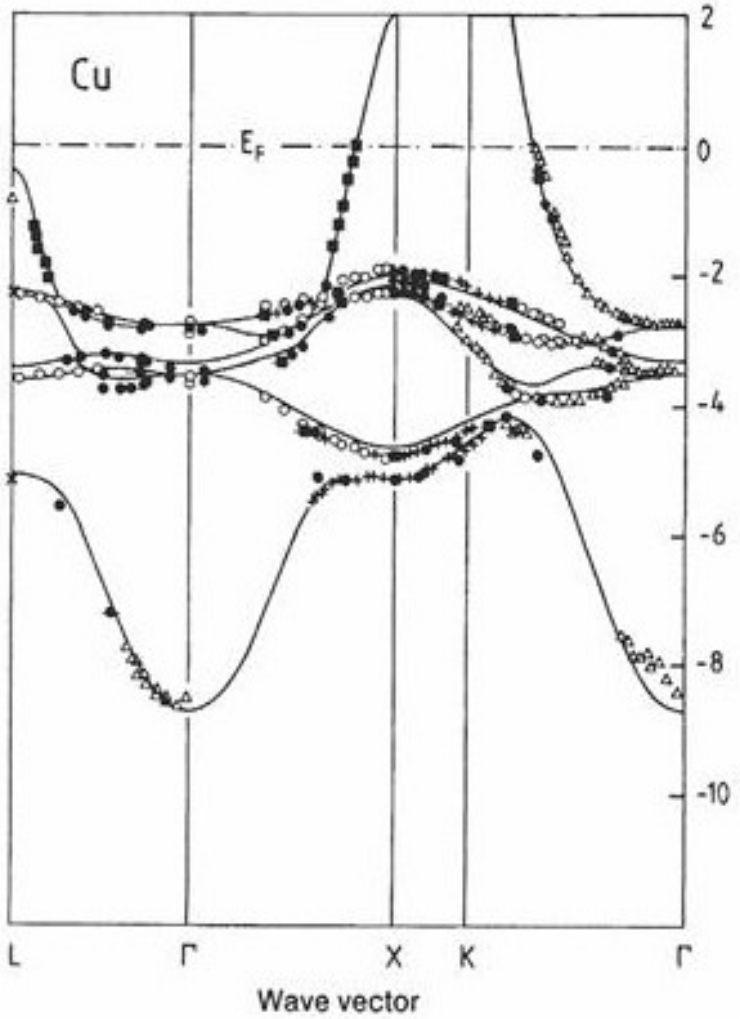
Optical absorption



Hydrogen Energy Level Diagram

Hydrogen atom

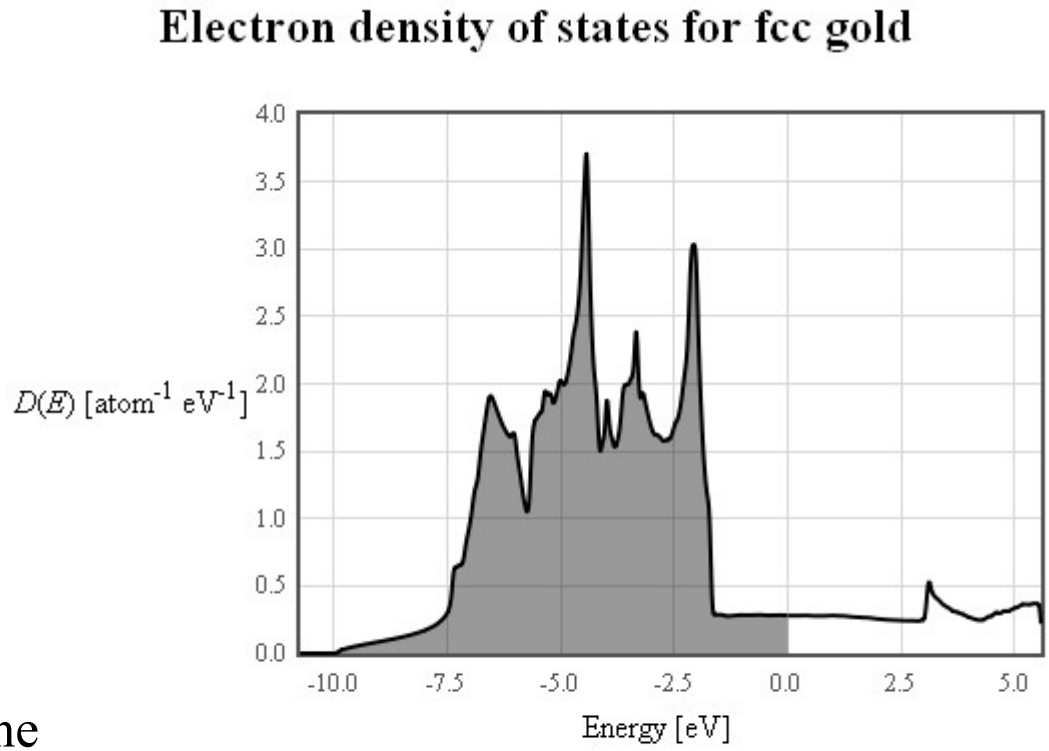




Copper fcc crystal

Thermodynamic properties of metals

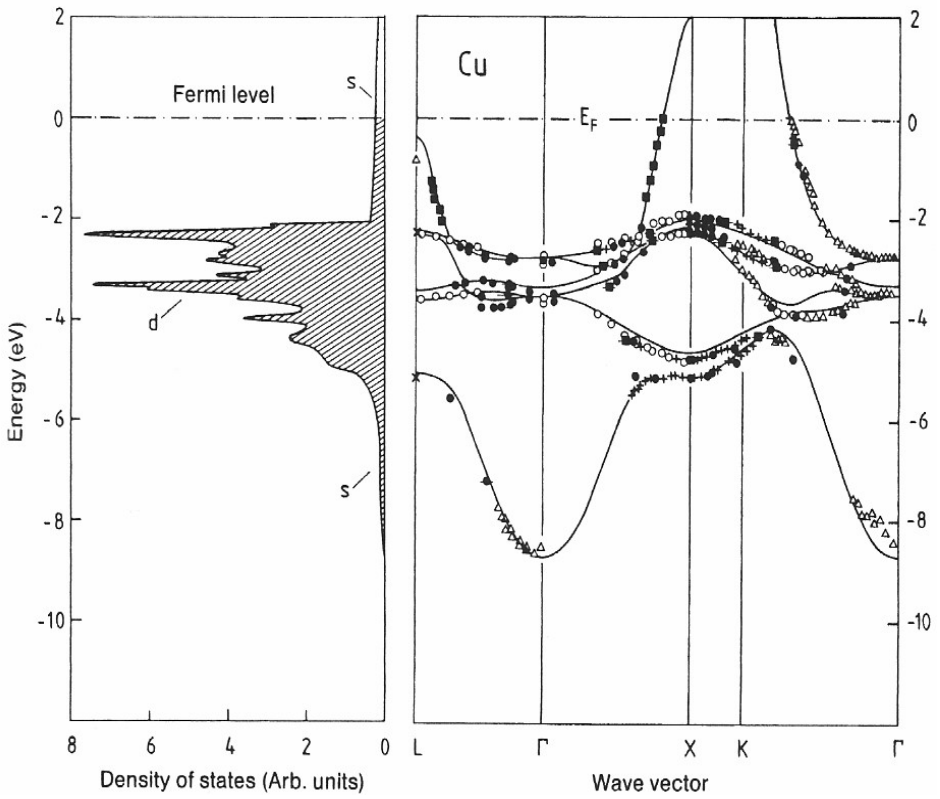
From the band structure measurements, we obtain the electron density of states.

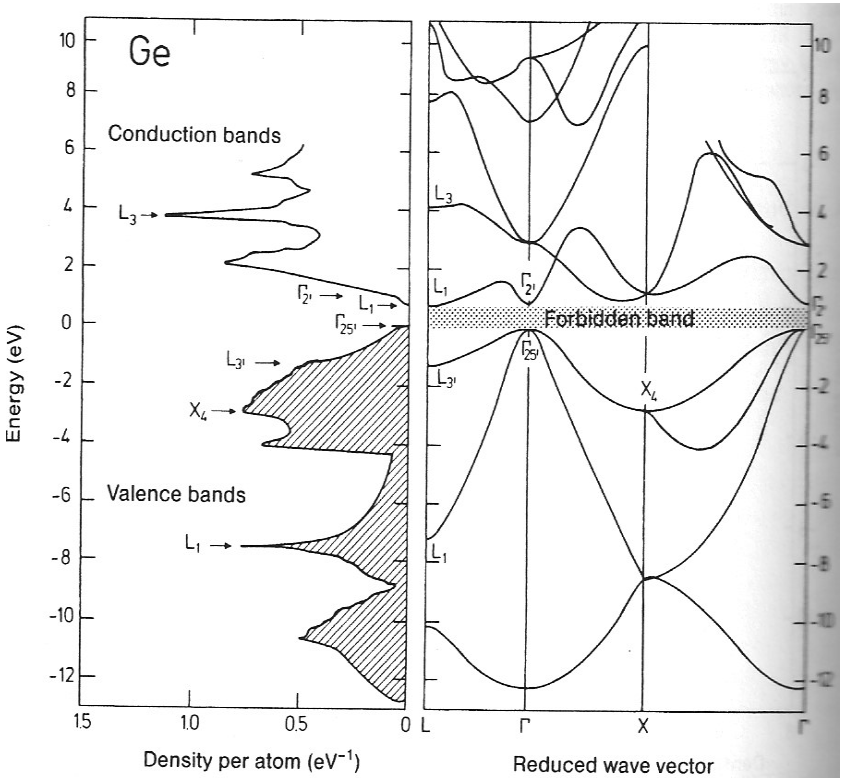


Thermodynamic properties can be calculated from the tabulated data for the density of states

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

Metals, semiconductors, and insulators





Insulators: band gap > 3 eV

From Ibach & Lueth