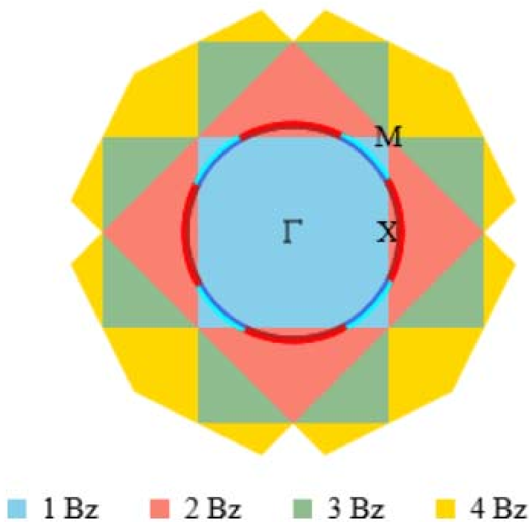
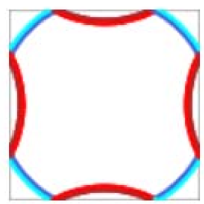
Fermi surface

2d square lattice

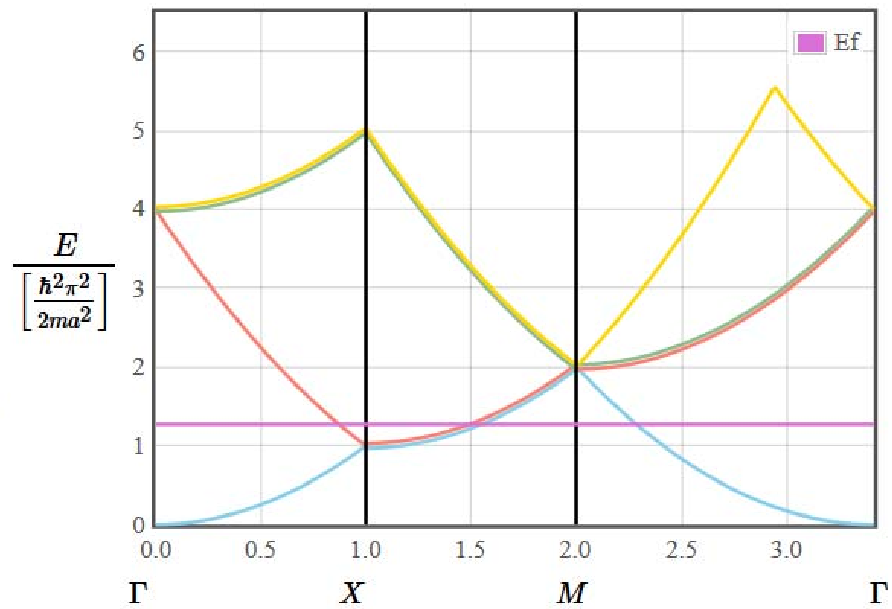
$2N$ electron states in a Brillouin zone



Extended Zone Scheme



Reduced Zone Scheme



The Fermi surface strikes the Brillouin zone boundary at 90°.

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

Brillouin zones of two-dimensional Bravais lattices

$$\vec{a}_1 = a\,\hat{x}, \qquad \vec{a}_2 = b\cos\gamma\,\hat{x} + b\sin\gamma\,\hat{y}.$$

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

$$\vec{b}_1 = \frac{2\pi}{a}\,\hat{k}_x - \frac{2\pi\cos\gamma}{a\sin\gamma}\,\hat{k}_y, \qquad \vec{b}_2 = \frac{2\pi}{b\sin\gamma}\,\hat{k}_y.$$

$$G_{hk,x} = hb_{1,x} + kb_{2,x} \text{ and } G_{hk,y} = hb_{1,y} + kb_{2,y}.$$

$$G_{hk,x}k_x + G_{hk,y}k_y = \frac{G^2_{hk,x}}{2} + \frac{G^2_{hk,y}}{2},$$

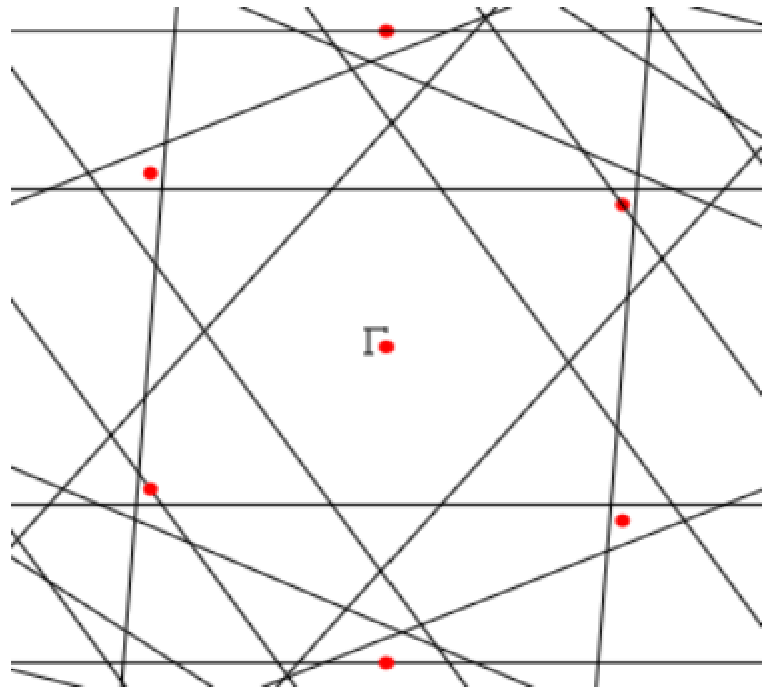
b/a =1.6 - +

γ =155 - +

square hexagonal

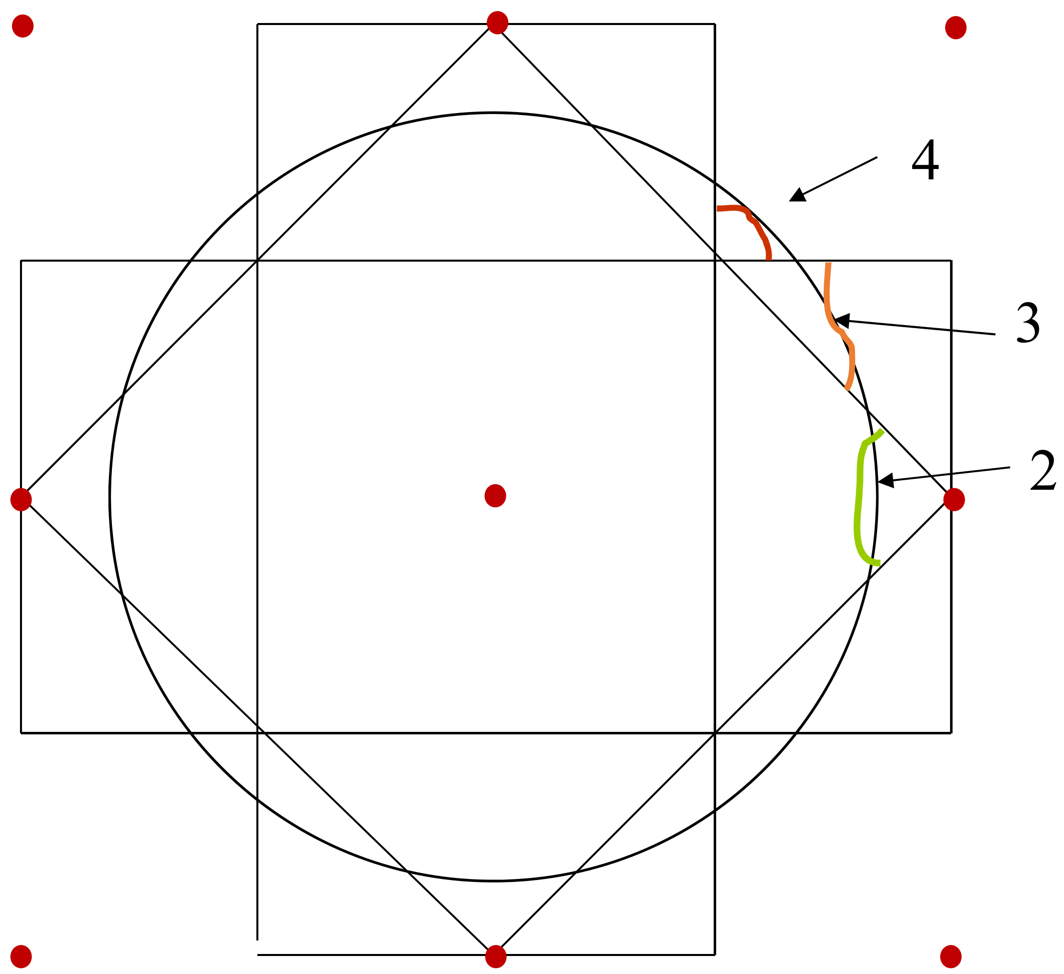
$\vec{a}_1 = 1\,\hat{x}$ $\qquad$ $\vec{a}_2 =$ -1.450 $\hat{x}$+(0.6762)$\hat{y}$

$\vec{b}_1 = 6.283\ \hat{k}_x$+(13.47)$\hat{k}_y$ $\qquad$ $\vec{b}_2 = 9.292\hat{k}_y$



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

Constructing Fermi surface



No Fermi surface in the 1st Brillouin zone

Fermi Surfaces

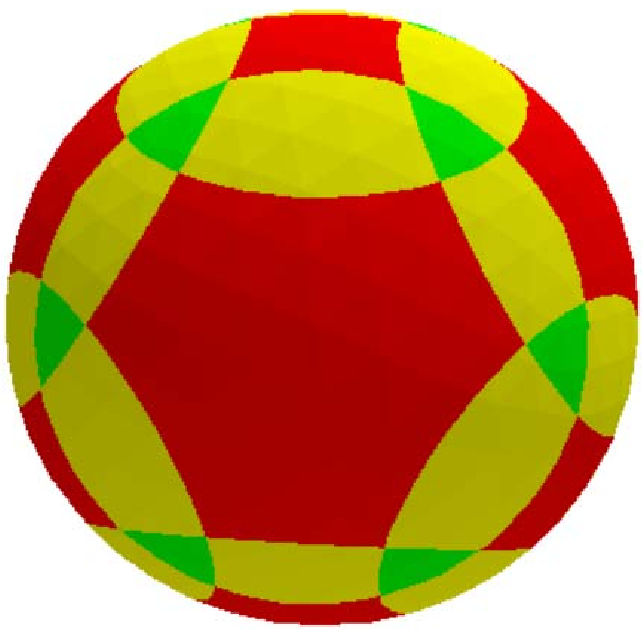
n =3.6 [-] [+] electrons/unit cell

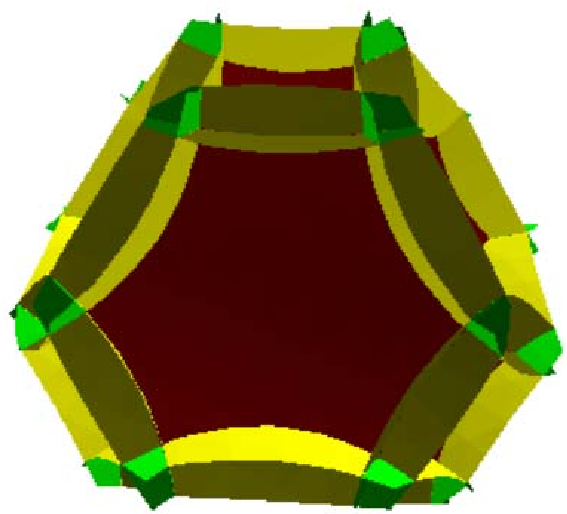
$$k_F = (3\pi^2 n)^{1/3} = 4.74$$

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

The thermodynamic properties of metals

Recipe for determining the thermodynamic properties of a metal

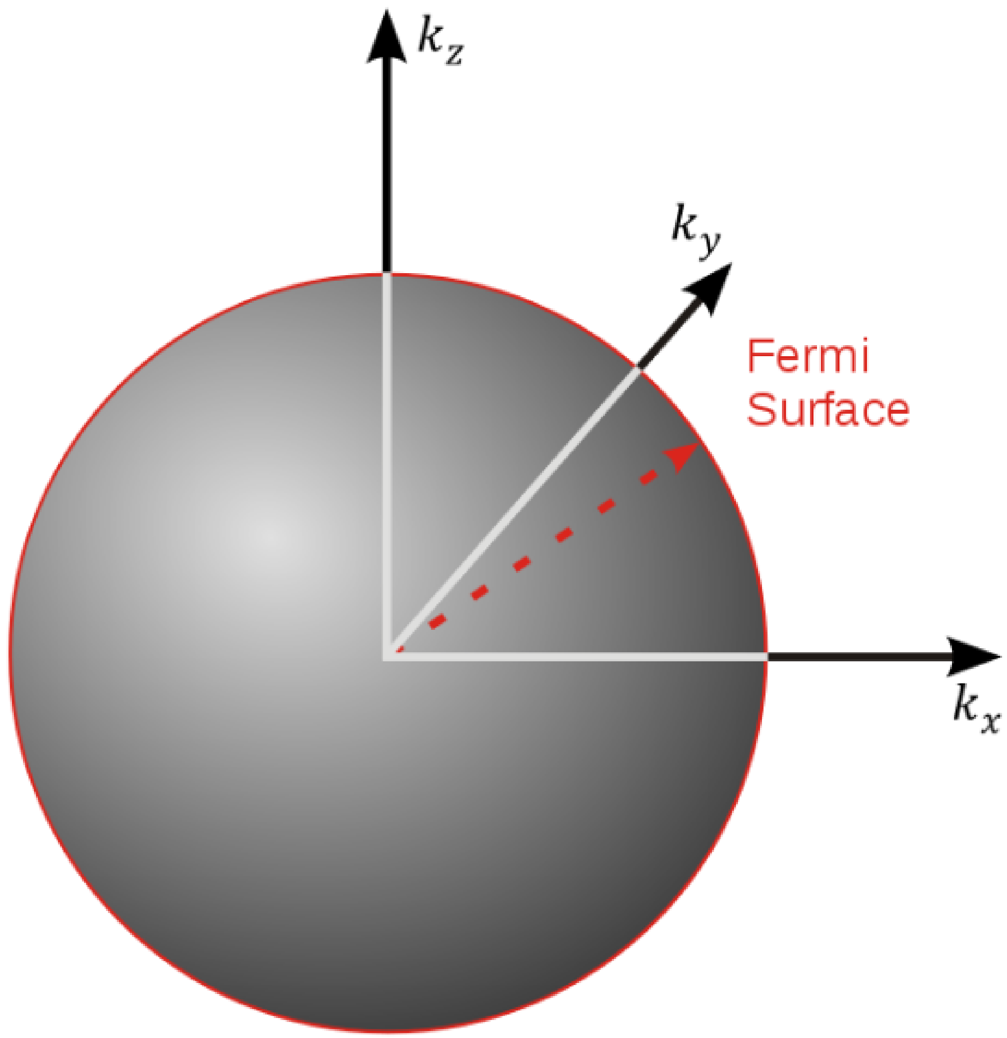
Solve the Schrödinger equation for an electrons moving in the periodic potential of the crystal

From the energy - k dispersion relation, determine the density of states.

Use the density of states to determine the thermodynamic properties

States near the Fermi surface determine the thermodynamic properties

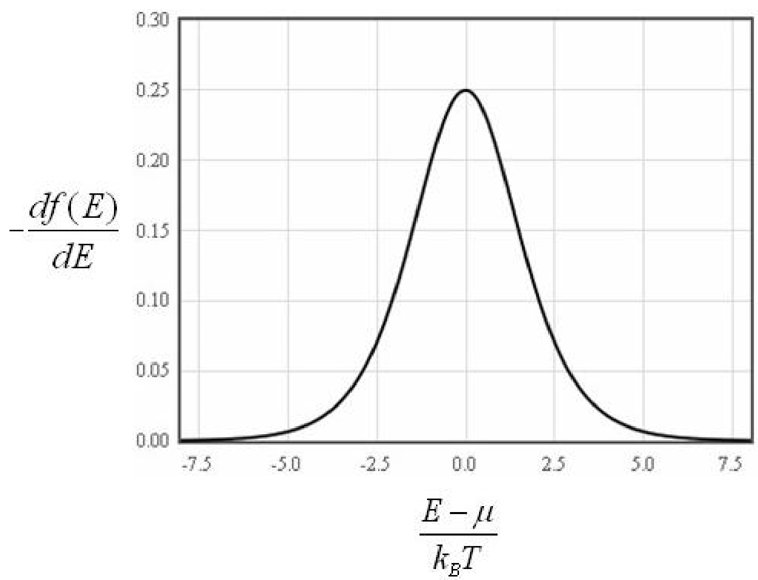
Fermi surface for free electrons



Properties of metals depend mostly on the electron states at the Fermi surface

$$n = \int_{-\infty}^{\infty} D(E) f(E) dE = \int_{-\infty}^{\infty} \frac{D(E) dE}{\exp\left(\frac{E-\mu}{k_B T}\right)+1}.$$

$$n = \int_{-\infty}^{\infty} D(E) f(E) dE = K(\infty) f(\infty) - K(-\infty) f(-\infty) - \int_{-\infty}^{\infty} K(E) \frac{f(E)}{dE} dE.$$



http://lampx.tugraz.at/~hadley/ss1/materials/thermo/dos2mu.html

Thermodynamic properties

Chemical potential (implicitly defined by):

$$n = \int_{-\infty}^{\infty} \frac{D(E)}{1+\exp\left(\frac{(E-\mu)}{k_BT}\right)} dE$$

DoS → mu

Internal energy density:

$$u = \phi + Ts + \mu n = \int_{-\infty}^{\infty} \frac{ED(E)}{1+\exp\left(\frac{E-\mu}{k_BT}\right)} dE$$

DoS → u(T)

Energy spectral density:

$$u(E,T) = \frac{ED(E)}{1+\exp\left(\frac{E-\mu}{k_BT}\right)}$$

DoS → u(E)

Specific heat:

$$c_v = \frac{\partial u}{\partial T} = \int_{-\infty}^{\infty} \frac{ED(E)(E-\mu)\exp\left(\frac{E-\mu}{k_BT}\right)}{k_BT^2\left(1+\exp\left(\frac{E-\mu}{k_BT}\right)\right)^2} dE$$

DoS → cv(T)

http://lamp.tu-graz.ac.at/~hadley/ss2/fermigas/thermo/thermo.php

Band structure calculations

Start with the full Hamiltonian.

$$H = -\sum_i \frac{\hbar^2}{2m_e}\nabla_i^2 - \sum_A \frac{\hbar^2}{2m_A}\nabla_A^2 - \sum_{i,A}\frac{Z_A e^2}{4\pi\varepsilon_0 r_{iA}} + \sum_{i<j}\frac{e^2}{4\pi\varepsilon_0 r_{ij}} + \sum_{A<B}\frac{Z_A Z_B e^2}{4\pi\varepsilon_0 r_{AB}}$$

Everything you can know is contained in this Hamiltonian.

Usually this is too difficult to solve.

http://en.wikipedia.org/wiki/File:Erwin_Schr%C3%B6dinger.jpg

Electrons in a crystal

Fix the positions of the nuclei (Born Oppenheimer approximation) and consider the many electron Hamiltonian.

$$H_{elec} = -\sum_i \frac{\hbar^2}{2m_e}\nabla_i^2 - \sum_{i,A}\frac{Z_A e^2}{4\pi\varepsilon_0 r_{iA}} + \sum_{i<j}\frac{e^2}{4\pi\varepsilon_0 r_{ij}}$$

This is still too difficult. Neglect the electron-electron interactions.

Separation of variables

$$H_{elec} = -\sum_i \frac{\hbar^2}{2m_e}\nabla_i^2 - \sum_{i,A}\frac{Z_A e^2}{4\pi\varepsilon_0 r_{iA}} + \cancel{\sum_{i<j}\frac{e^2}{4\pi\varepsilon_0 r_{ij}}}$$

The electronic Hamiltonian separates into the molecular orbital Hamiltonians.

$H_{\mathrm{elec}}(\mathrm{r}_1,\mathrm{r}_2,\ldots\mathrm{r}_n) = H_{\mathrm{MO}}(\mathrm{r}_1) + H_{\mathrm{MO}}(\mathrm{r}_2) + \ldots\ H_{\mathrm{MO}}(\mathrm{r}_n)$

$\Psi_{\mathrm{elec}}(\mathrm{r}_1,\mathrm{r}_2,\ldots\mathrm{r}_n) = |\psi_{\mathrm{MO}}(\mathrm{r}_1)\psi_{\mathrm{MO}}(\mathrm{r}_2)\ \ldots\ \psi_{\mathrm{MO}}(\mathrm{r}_n)>$

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

Solving the molecular orbital Hamiltonian

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

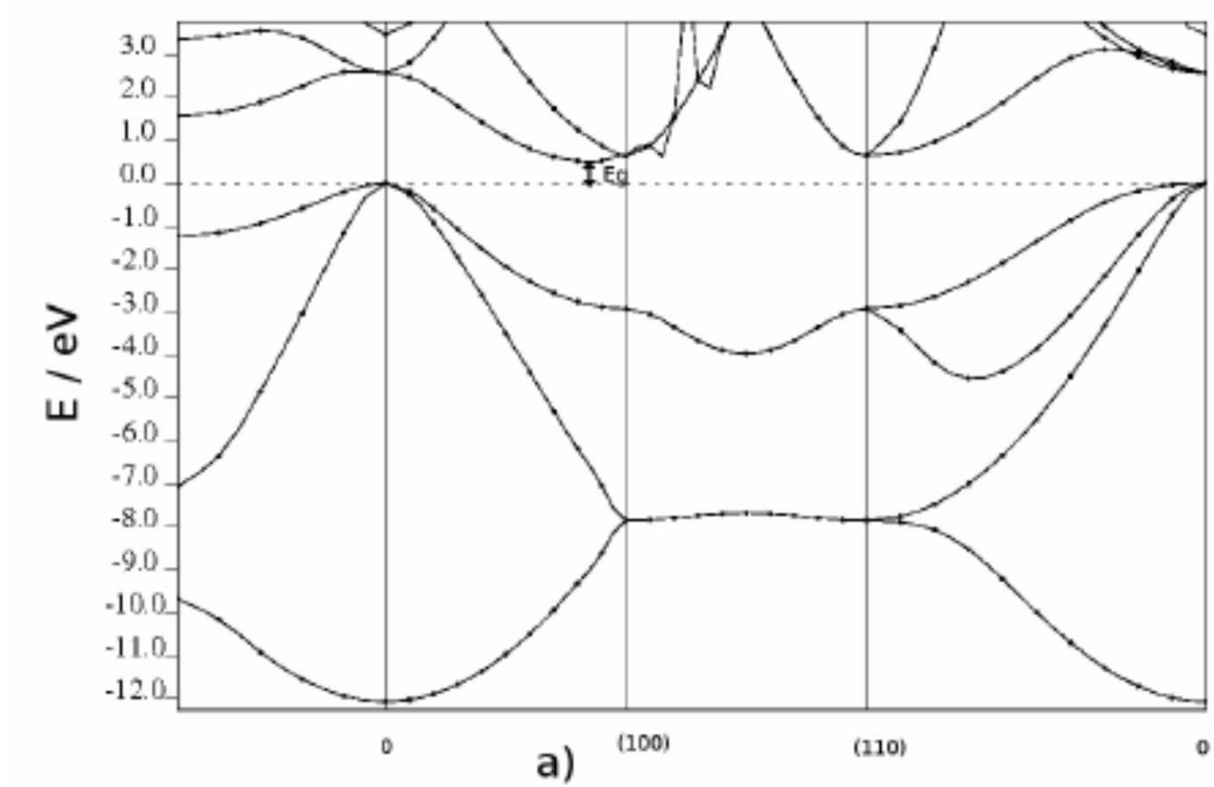
Band structure calculations:

Plane wave method
Tight binding (LCAO+)

DFT

Si

Bachelor thesis Benedikt Tschofenig



QUANTUMESPRESSO

http://www.quantum-espresso.org/

Plane wave method

$$-\frac{\hbar^2}{2m}\nabla^2\psi + U_{MO}(\vec{r})\psi = E\psi$$

Write U and ψ as Fourier series.

$$U_{MO}(\vec{r}) = \sum_{\vec{G}} U_{\vec{G}} e^{i\vec{G}\cdot\vec{r}} \qquad\qquad \psi(\vec{r}) = \sum_{\vec{k}} C_{\vec{k}} e^{i\vec{k}\cdot\vec{r}}$$

For the molecular orbital Hamiltonian

$$U_{MO}(\vec{r}) = \frac{-Ze^2}{4\pi\varepsilon_0}\sum_j \frac{1}{\left|\vec{r}-\vec{r}_j\right|} = \frac{-Ze^2}{V\varepsilon_0}\sum_{\vec{G}} \frac{e^{i\vec{G}\cdot\vec{r}}}{G^2}$$

volume of a unit cell

Plane wave method

$$-\frac{\hbar^2}{2m}\nabla^2\psi + U(\vec{r})\psi = E\psi$$

$$U_{MO}(\vec{r}) = \sum_{\vec{G}} U_{\vec{G}} e^{i\vec{G}\cdot\vec{r}} \qquad \psi(\vec{r}) = \sum_{\vec{k}} C_{\vec{k}} e^{i\vec{k}\cdot\vec{r}}$$

$$\sum_{\vec{k}} \frac{\hbar^2 k^2}{2m} C_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} + \sum_{\vec{G}} \sum_{\vec{k}'} U_{\vec{G}} C_{\vec{k}'} e^{i(\vec{G}+\vec{k}')\cdot\vec{r}} = E \sum_{\vec{k}} C_{\vec{k}} e^{i\vec{k}\cdot\vec{r}}$$

Must hold for each Fourier coefficient.

$$\vec{k}' + \vec{G} = \vec{k} \quad \Rightarrow \quad \vec{k}' = \vec{k} - \vec{G}$$

$$\boxed{\left(\frac{\hbar^2 k^2}{2m} - E\right) C_{\vec{k}} + \sum_{\vec{G}} U_{\vec{G}} C_{\vec{k}-\vec{G}} = 0}$$

Central equations (one for every k in the first Brillouin zone)

Plane wave method

The central equations can be written as a matrix equation.

$$M\vec{C} = E\vec{C}$$

Diagonal elements: $$M_{ii} = \frac{\hbar^2}{2m}\left(\vec{k} - \vec{G}_i\right)^2$$

Off-diagonal elements: $$M_{ij} = -\frac{Ze^2}{V\varepsilon_0\left(\vec{G}_i - \vec{G}_j\right)^2}$$

Central equations - one dimension

$$\boxed{\left(\frac{\hbar^2 k^2}{2m} - E\right) C_k + \sum_G U_G C_{k-G} = 0}$$

$$\begin{bmatrix} \ddots & & & & & \\ \frac{\hbar^2 (k-2G_0)^2}{2m} - E & U_{G_0} & U_{2G_0} & U_{3G_0} & U_{4G_0} & U_{5G_0} \\ U_{-G_0} & \frac{\hbar^2 (k-G_0)^2}{2m} - E & U_{G_0} & U_{2G_0} & U_{3G_0} & U_{4G_0} \\ U_{-2G_0} & U_{-G_0} & \frac{\hbar^2 k^2}{2m} - E & U_{G_0} & U_{2G_0} & U_{3G_0} \\ U_{-3G_0} & U_{-2G_0} & U_{-G_0} & \frac{\hbar^2 (k+G_0)^2}{2m} - E & U_{G_0} & U_{2G_0} \\ U_{-4G_0} & U_{-3G_0} & U_{-2G_0} & U_{-G_0} & \frac{\hbar^2 (k+2G_0)^2}{2m} - E & U_{G_0} \\ & & & & & \ddots \end{bmatrix} \begin{bmatrix} \vdots \\ C_{k+2G_0} \\ C_{k+G_0} \\ C_k \\ C_{k-G_0} \\ C_{k-2G_0} \\ \vdots \end{bmatrix} = 0$$

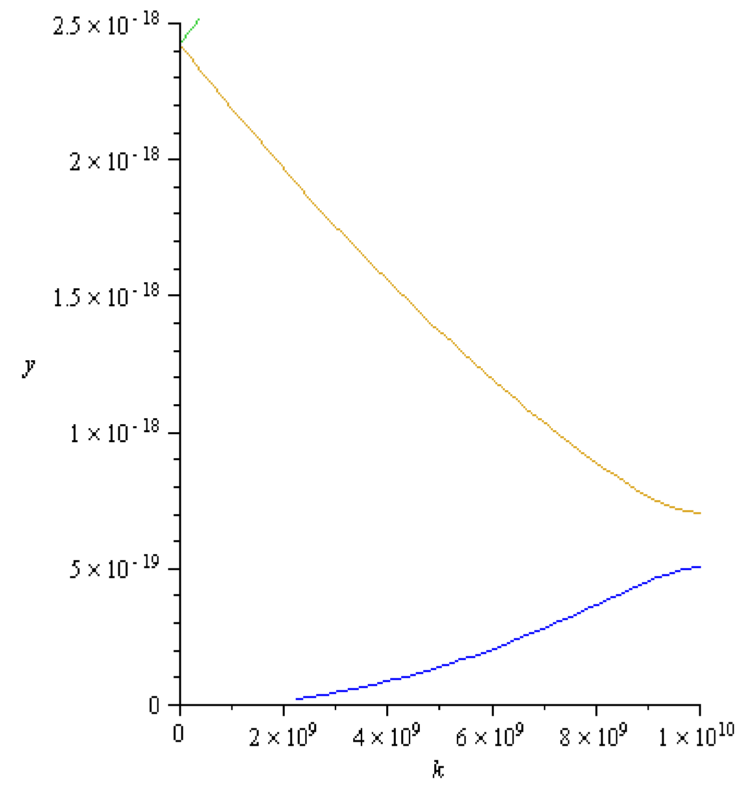
Central equations couple coefficients k to other coefficients that differ by a reciprocal lattice wavevector G.

Central equations - one dimension

$$M4 := \begin{bmatrix} \frac{\mathrm{hbar}^2\cdot(k+2\cdot G)^2}{2m} & \mathrm{U} & 0 & 0 \\ \mathrm{U} & \frac{\mathrm{hbar}^2\cdot(k+G)^2}{2m} & U & 0 \\ 0 & U & \frac{\mathrm{hbar}^2\cdot k^2}{2m} & U \\ 0 & 0 & U & \frac{\mathrm{hbar}^2\cdot(k-G)^2}{2m} \end{bmatrix}:$$

$V4 := Eigenvalues(M4):$

$plot([V4[1], V4[2], V4[3], V4[4]], k = 0..1E10, y = 0..2.5E-18);$



Central equations 3d - simple cubic

$$V(\vec{r}) = \sum_{\vec{G}} U_{\vec{G}} e^{i\vec{G}\cdot\vec{r}}$$

Molecular orbital Hamiltonian

$$U_{\vec{G}} = \frac{-Ze^2}{V_{\text{unit cell}}\varepsilon_0 G^2}$$

Central equations: $$\left(\frac{\hbar^2 k^2}{2m} - E\right) C_{\vec{k}} + \sum_{\vec{G}} U_{\vec{G}} C_{\vec{k}-\vec{G}} = 0$$

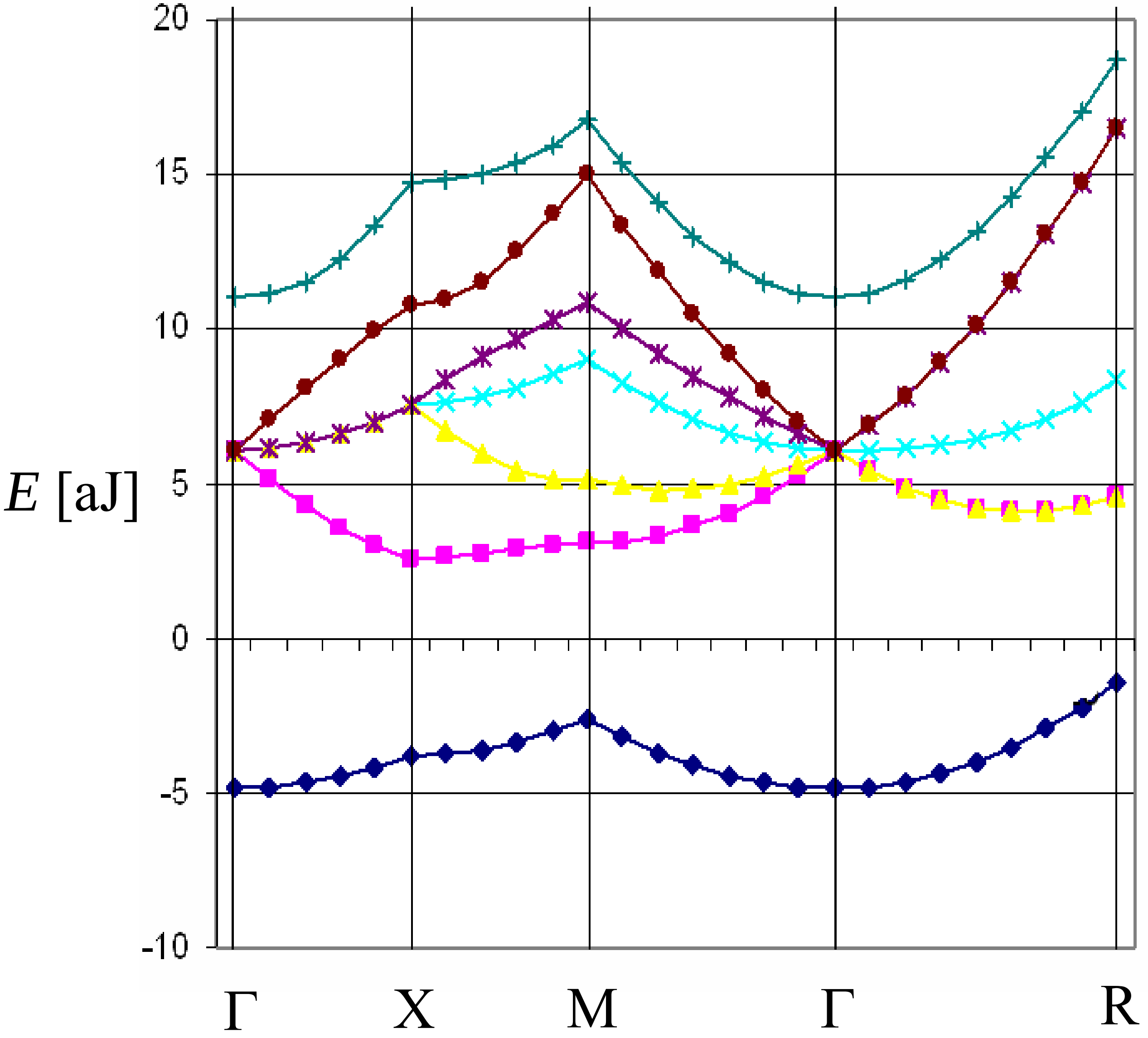
diagonal elements: $$\frac{\hbar^2}{2m}\left(\vec{k} - \vec{G}_i\right)^2$$

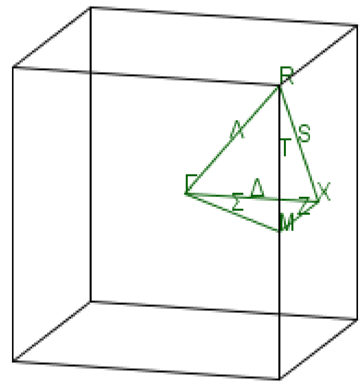
off-diagonal elements: $$\frac{-Ze^2}{V_{\text{unit cell}}\varepsilon_0 \left(\vec{G}_i - \vec{G}_j\right)^2}$$

Central equations - simple cubic

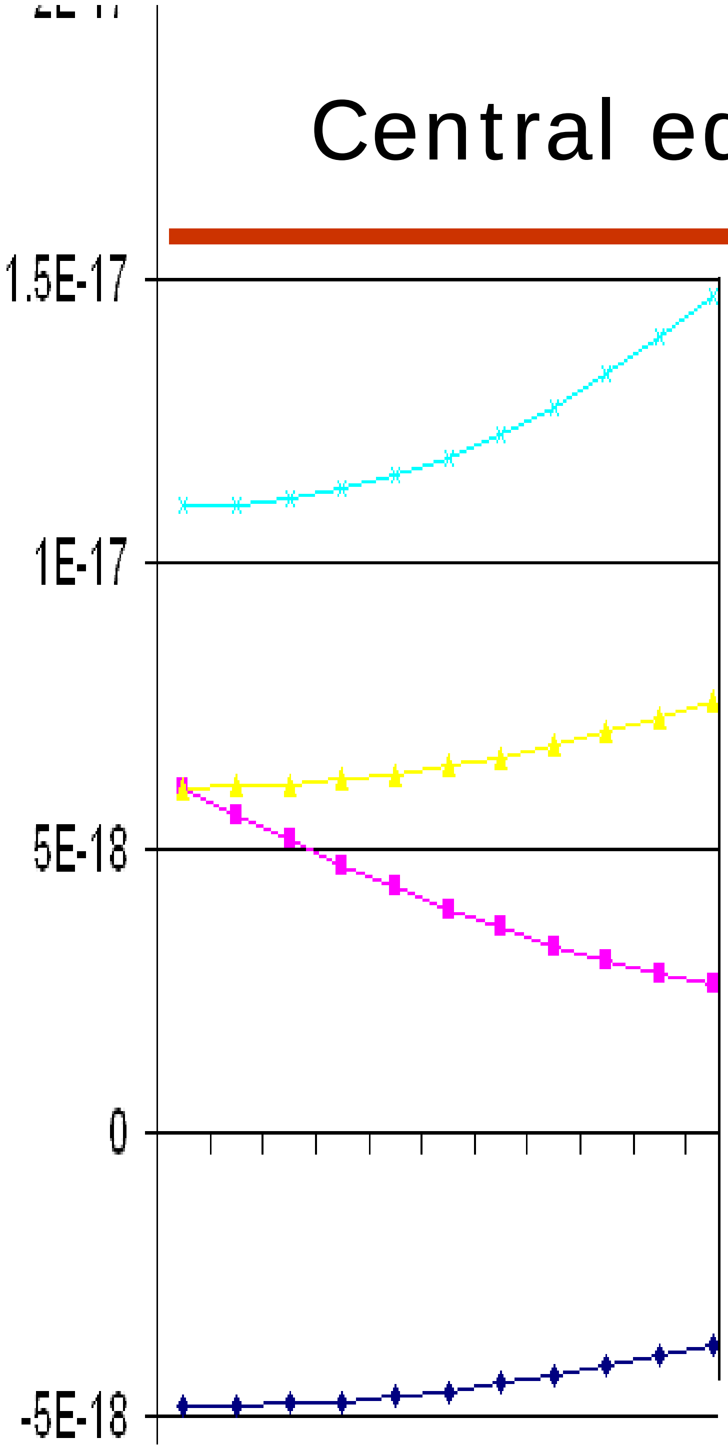
$$
\begin{pmatrix}
\frac{\hbar^2\left(\vec{k}+\frac{2\pi}{a}\hat{k}_z\right)^2}{2m} & \frac{-Ze^2a^2}{8V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{-Ze^2a^2}{8V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{-Ze^2a^2}{4V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{-Ze^2a^2}{8V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{-Ze^2a^2}{8V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{-Ze^2a^2}{16V_{\text{unit cell}}\varepsilon_0\pi^2} \\
\frac{-Ze^2a^2}{8V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{\hbar^2\left(\vec{k}+\frac{2\pi}{a}\hat{k}_y\right)^2}{2m} & \frac{-Ze^2a^2}{8V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{-Ze^2a^2}{4V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{-Ze^2a^2}{8V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{-Ze^2a^2}{16V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{-Ze^2a^2}{8V_{\text{unit cell}}\varepsilon_0\pi^2} \\
\frac{-Ze^2a^2}{8V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{-Ze^2a^2}{8V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{\hbar^2\left(\vec{k}+\frac{2\pi}{a}\hat{k}_x\right)^2}{2m} & \frac{-Ze^2a^2}{4V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{-Ze^2a^2}{16V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{-Ze^2a^2}{8V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{-Ze^2a^2}{8V_{\text{unit cell}}\varepsilon_0\pi^2} \\
\frac{-Ze^2a^2}{4V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{-Ze^2a^2}{4V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{-Ze^2a^2}{4V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{\hbar^2k^2}{2m} & \frac{-Ze^2a^2}{4V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{-Ze^2a^2}{4V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{-Ze^2a^2}{4V_{\text{unit cell}}\varepsilon_0\pi^2} \\
\frac{-Ze^2a^2}{8V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{-Ze^2a^2}{8V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{-Ze^2a^2}{16V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{-Ze^2a^2}{4V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{\hbar^2\left(\vec{k}-\frac{2\pi}{a}\hat{k}_x\right)^2}{2m} & \frac{-Ze^2a^2}{8V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{-Ze^2a^2}{8V_{\text{unit cell}}\varepsilon_0\pi^2} \\
\frac{-Ze^2a^2}{8V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{-Ze^2a^2}{16V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{-Ze^2a^2}{8V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{-Ze^2a^2}{4V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{-Ze^2a^2}{8V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{\hbar^2\left(\vec{k}-\frac{2\pi}{a}\hat{k}_y\right)^2}{2m} & \frac{-Ze^2a^2}{8V_{\text{unit cell}}\varepsilon_0\pi^2} \\
\frac{-Ze^2a^2}{16V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{-Ze^2a^2}{2V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{-Ze^2a^2}{8V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{-Ze^2a^2}{4V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{-Ze^2a^2}{8V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{-Ze^2a^2}{8V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{\hbar^2\left(\vec{k}-\frac{2\pi}{a}\hat{k}_z\right)^2}{2m}
\end{pmatrix}
$$

Central equations - simple cubic

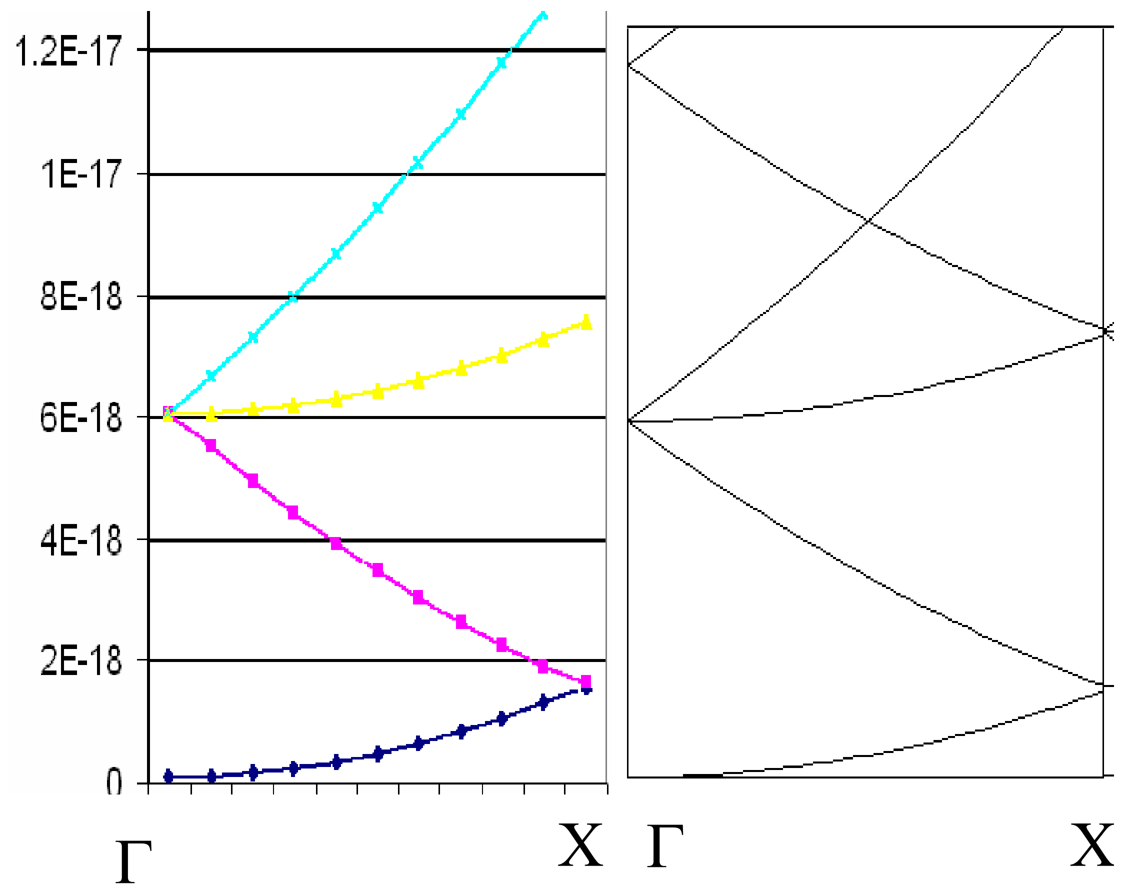




Central equations - simple cubic



empty lattice



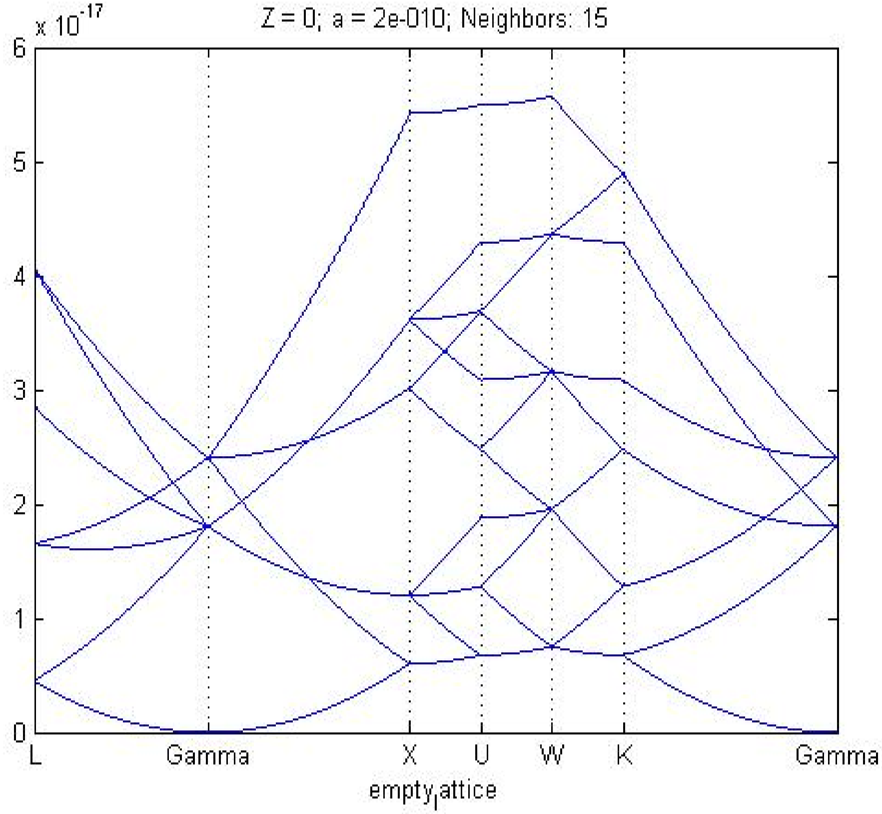
Plane wave method

Editor - I:\planewave\fcc_plane_wave_script.m

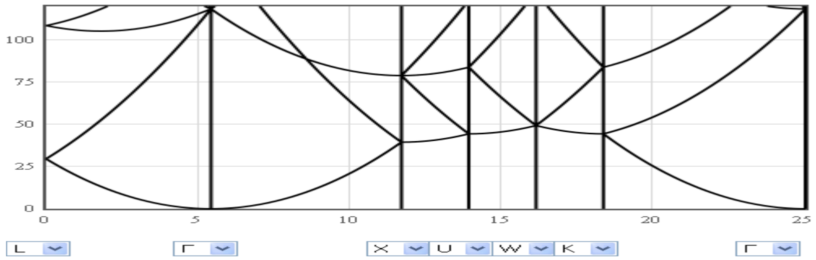
```matlab
% clc
clear all
%close all % comment with % if you would like to compare some results
tic

% constants in si units

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%



% change to a any value
% be sure that 'other' is selected as metal
Z = 6; % atomic number
a = 2E-10; % lattice constant a

% choose 'other' to use the assigned values for Z and a from above
% choose 'copper' 'silver' 'gold' 'aluminium' 'calcium' or 'lead' to use
% preset values
metal = 'aluminum';

dist_neighbors = 3; % only nearest neighbors = 1 ; nearest and next nearest = 2 etc.
% maximum is 1136. However at high numbers some neighbors are missed


%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%


switch lower(metal)
    case 'copper'
        Z = 29;
        a = 3.61e-10;
    case 'silver'
        Z = 47;
```

Plane wave method

fcc $Z = 0$

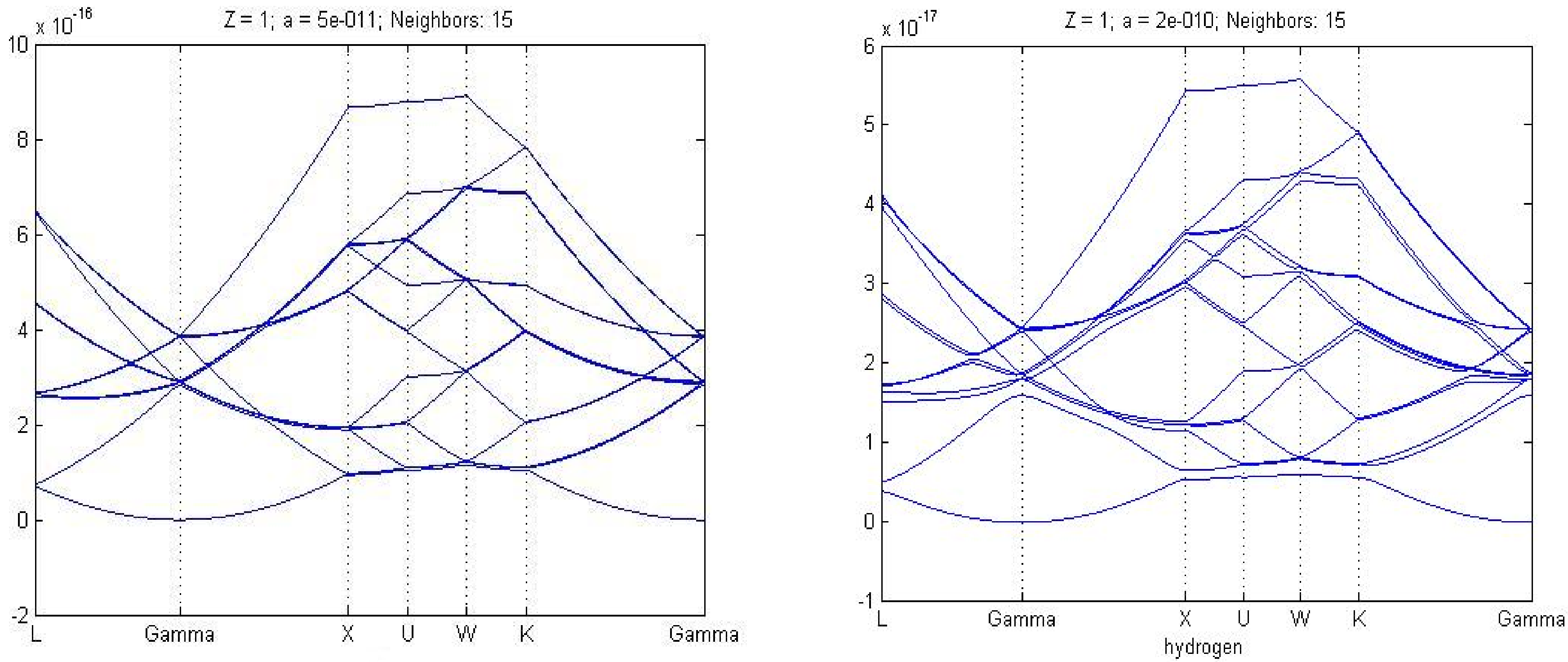


empty lattice



Plane wave method

fcc hydrogen



Approximate solution near the Bz boundary

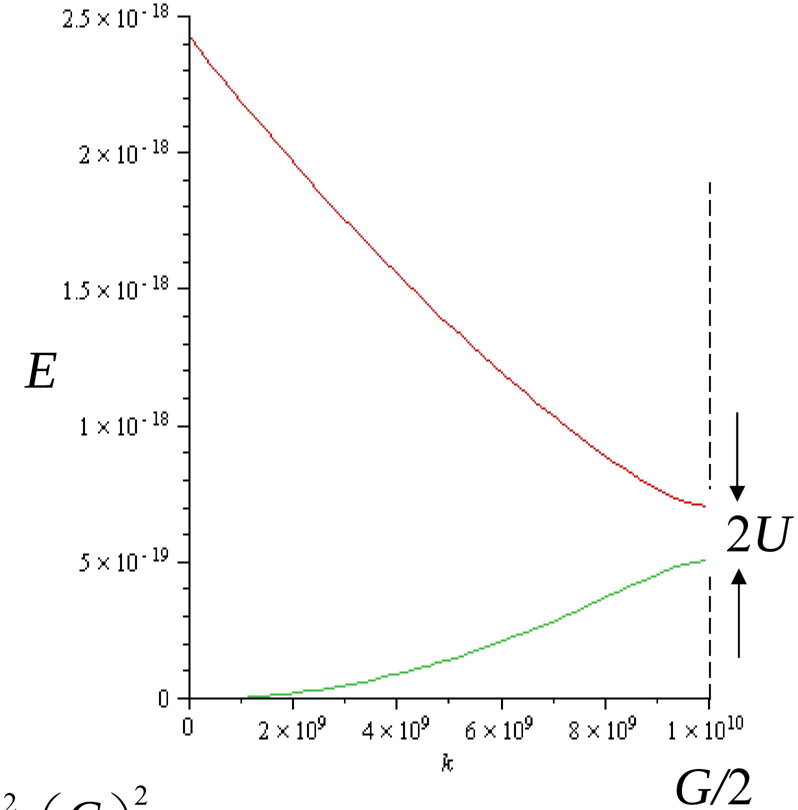
$$\boxed{\left(\frac{\hbar^2 k^2}{2m} - E\right) C_k + \sum_G U_G C_{k-G} = 0}$$

For just 2 terms

$$\begin{bmatrix} \frac{\hbar^2 k^2}{2m} - E & U \\ U & \frac{\hbar^2 (k-G)^2}{2m} - E \end{bmatrix} \begin{bmatrix} C_k \\ C_{k+G} \end{bmatrix} = 0$$

Near the Brillouin zone boundary $k \sim G/2$

$$\begin{bmatrix} \frac{\hbar^2}{2m}\left(\frac{G}{2}\right)^2 - E & U \\ U & \frac{\hbar^2}{2m}\left(\frac{G}{2}\right)^2 - E \end{bmatrix} \begin{bmatrix} C_k \\ C_{k+G} \end{bmatrix} = 0$$



$$E = \frac{\hbar^2}{2m}\left(\frac{G}{2}\right)^2 \pm U$$

Tight binding

Tight binding does not include electron-electron interactions

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

Assume a solution of the form.

$$\psi_k = \sum_{l,m,n} \exp\left(i\left(l\vec{k}\cdot\vec{a}_1 + m\vec{k}\cdot\vec{a}_2 + n\vec{k}\cdot\vec{a}_3\right)\right)\sum_a c_a\phi_a\left(\vec{r} - l\vec{a}_1 - m\vec{a}_2 - n\vec{a}_3\right)$$

atomic orbitals:
choose the relevant
valence orbitals

http://lamp.tu-graz.ac.at/~hadley/ss1/bands/tightbinding/tightbinding.php

Tight binding

$$\psi_k = \sum_{l,m,n} \exp\left(i\left(l\vec{k}\cdot\vec{a}_1 + m\vec{k}\cdot\vec{a}_2 + n\vec{k}\cdot\vec{a}_3\right)\right)\sum_a c_a\phi_a\left(\vec{r} - l\vec{a}_1 - m\vec{a}_2 - n\vec{a}_3\right)$$

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

$$\left\langle \phi_a \middle| H_{MO} \middle| \psi_k \right\rangle = E_k \left\langle \psi_a \middle| \psi_k \right\rangle$$

$$c_a \left\langle \phi_a \middle| H_{MO} \middle| \phi_a \right\rangle + \sum_{\text{nearest neighbors } m} c_m \left\langle \phi_a \middle| H_{MO} \middle| \phi_m \right\rangle \exp(i(h\vec{k}\cdot\vec{a}_1 + j\vec{k}\cdot\vec{a}_2 + l\vec{k}\cdot\vec{a}_3)) + \text{small terms}$$
$$= E_k c_a \left\langle \phi_a \middle| \phi_a \right\rangle + \text{small terms}$$

There is one equation for each atomic orbital

Tight binding, one atomic orbital

$$c_a \langle \phi_a | H_{MO} | \phi_a \rangle + \sum_{\text{nearest neighbors } m} c_m \langle \phi_a | H_{MO} | \phi_m \rangle \exp(i(h\vec{k}\cdot\vec{a}_1 + j\vec{k}\cdot\vec{a}_2 + l\vec{k}\cdot\vec{a}_3)) + \text{small terms}$$

$$= E_k c_a \langle \phi_a | \phi_a \rangle + \text{small terms}$$

For only one atomic orbital in the sum over valence orbitals

$$E_k c_a \langle \phi_a | \phi_a \rangle = c_a \langle \phi_a | H_{MO} | \phi_a \rangle + \sum_{\text{nearest neighbors } m} c_a \langle \phi_a | H_{MO} | \phi_m \rangle \exp(i(h\vec{k}\cdot\vec{a}_1 + j\vec{k}\cdot\vec{a}_2 + l\vec{k}\cdot\vec{a}_3))$$

one atomic orbital
$E_k = \varepsilon - t\sum_m e^{i\vec{k}\cdot\vec{\rho}_m}$

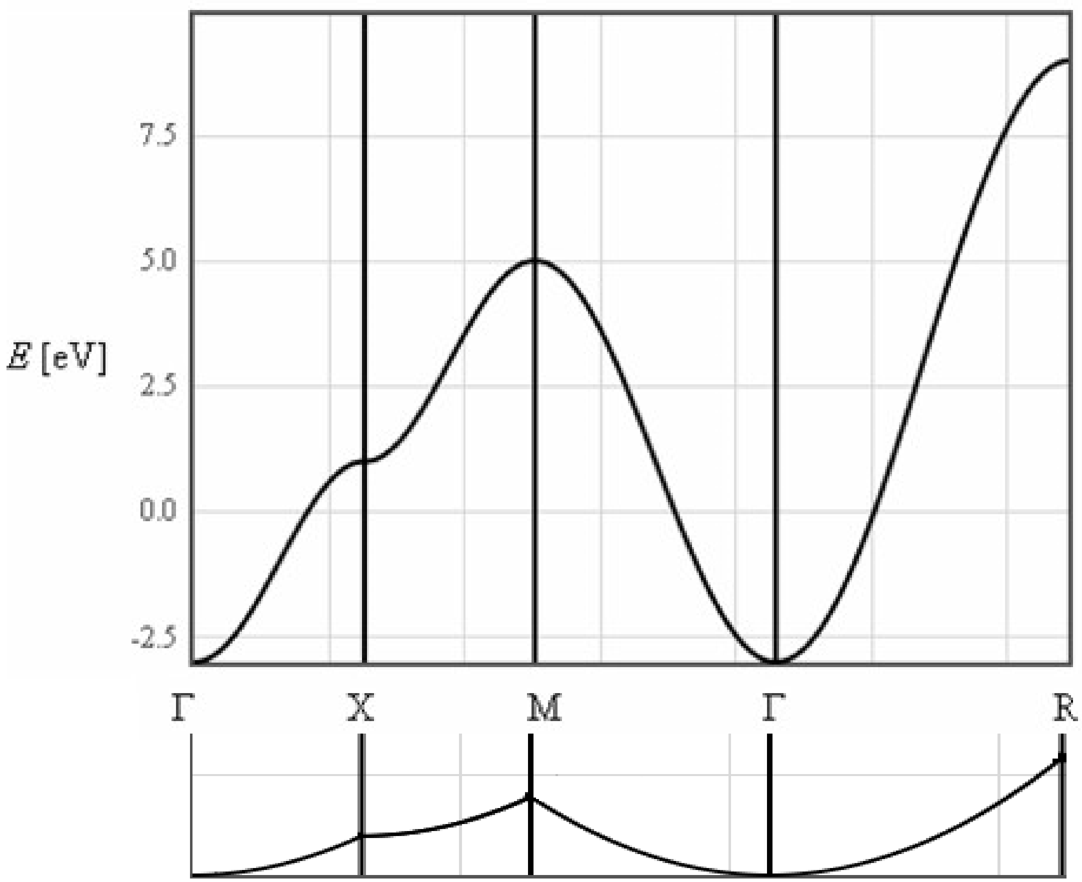
$$\varepsilon = \left\langle \phi_a(\vec{r}) \middle| H_{MO} \middle| \phi_a(\vec{r}) \right\rangle \qquad t = -\left\langle \phi_a(\vec{r}) \middle| H_{MO} \middle| \phi_a(\vec{r} - \vec{\rho}_m) \right\rangle$$

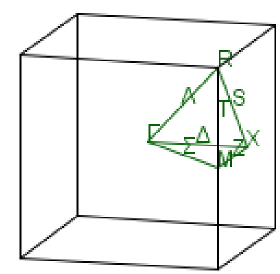
Tight binding, simple cubic

$$E = \varepsilon - t\sum_m e^{i\vec{k}\cdot\vec{\rho}_m}$$

$$E = \varepsilon - t\left(e^{ik_xa} + e^{-ik_xa} + e^{ik_ya} + e^{-ik_ya} + e^{ik_za} + e^{-ik_za}\right)$$

$$= \varepsilon - 2t\left(\cos(k_xa) + \cos(k_ya) + \cos(k_za)\right)$$

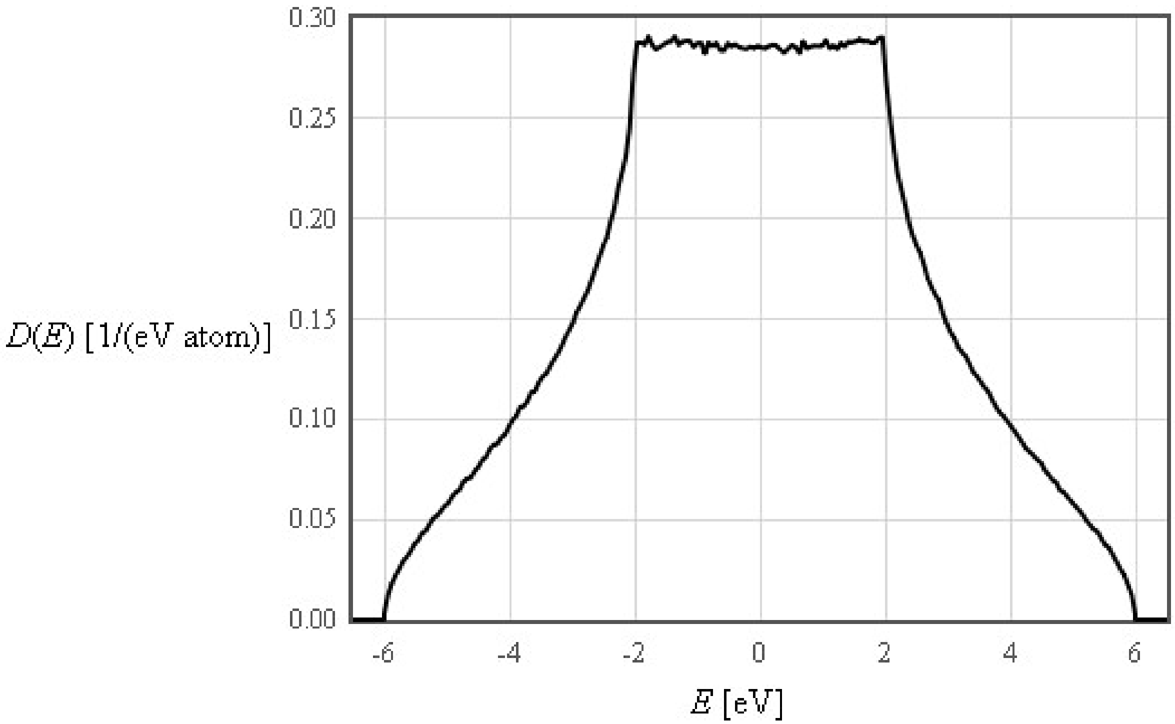




Effective mass $m^* = \frac{\hbar^2}{\frac{d^2E}{dk^2}} = \frac{\hbar^2}{2ta^2}$

Narrow bands → high effective mass

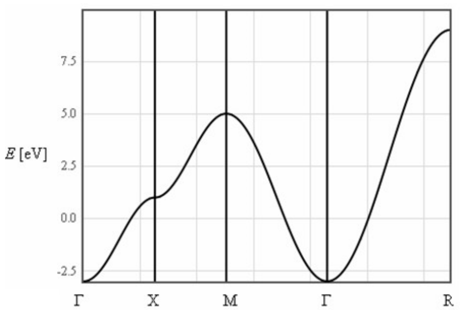
Density of states (simple cubic)



Calculate the energy for every allowed k in the Brillouin zone

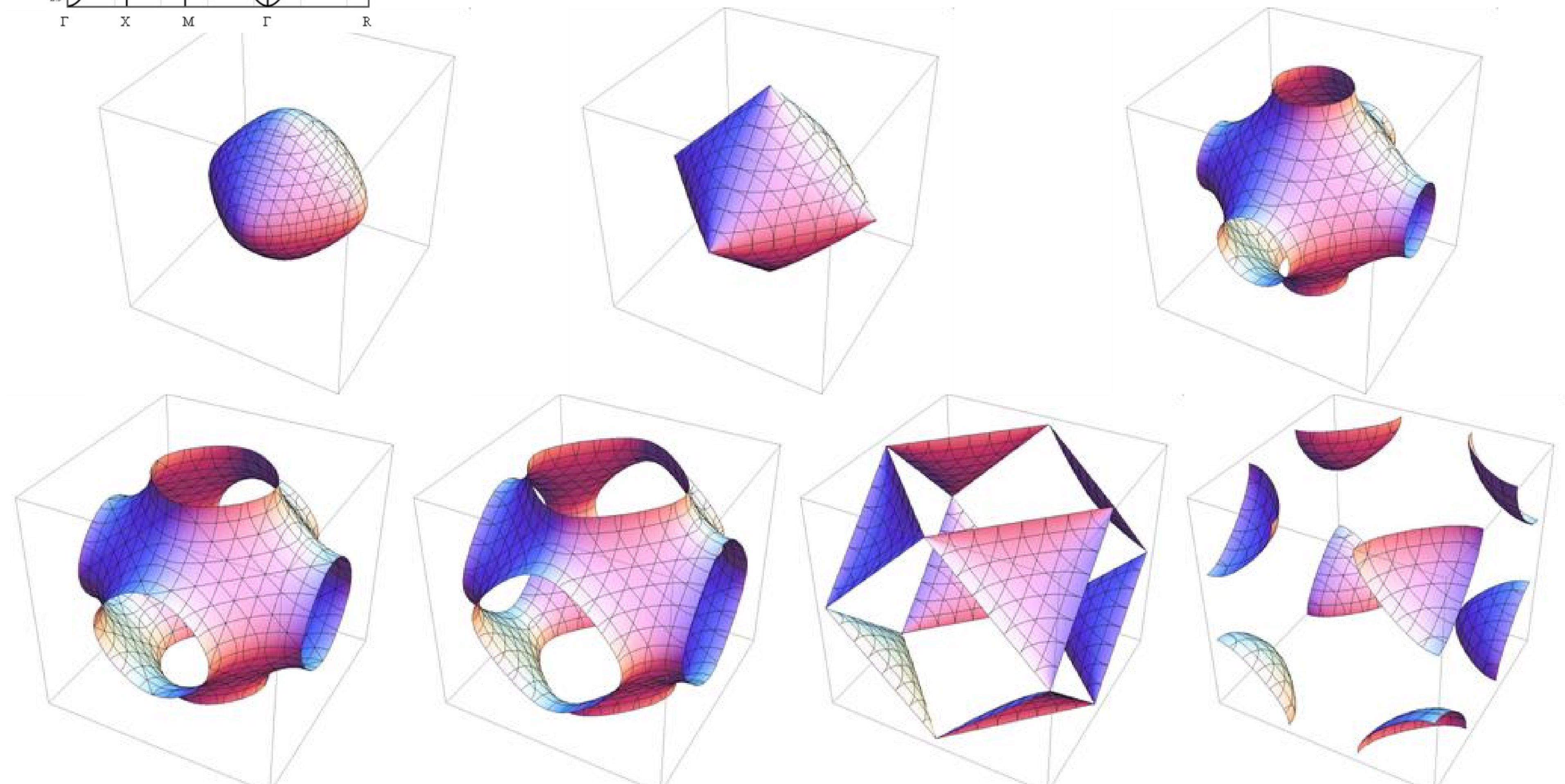
$$E = \varepsilon - 2t\left(\cos(k_x a) + \cos(k_y a) + \cos(k_z a)\right)$$

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



Tight binding, simple cubic

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



Christian Gruber, 2008