Electron bands

Plane wave method

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

Write U and ψ as Fourier series.

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

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.

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

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

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

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

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

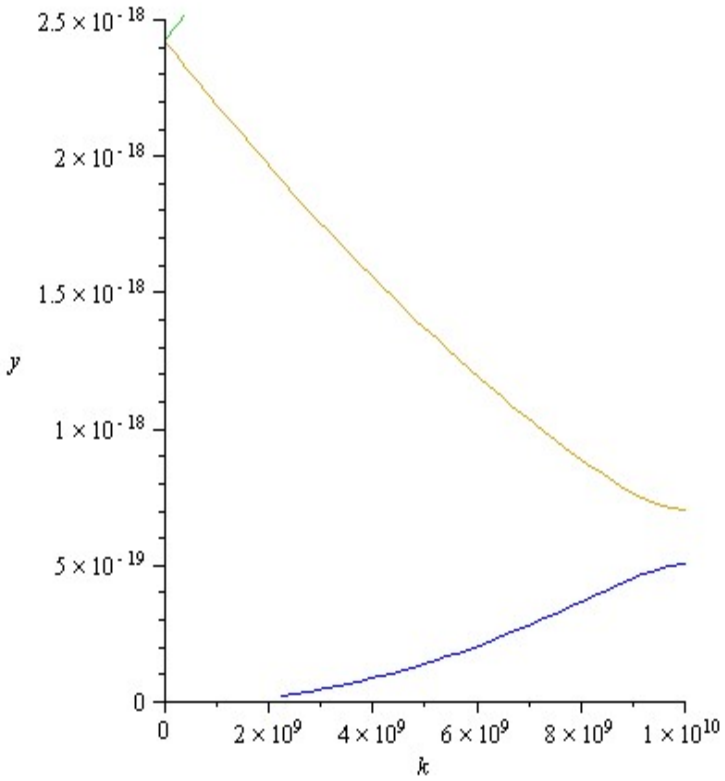
Central equations couple coefficients k to other coefficients that differ by a reciprocal lattice wavevector G.

Central equations - one dimension

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

$V4 := Eigenvalues(M4)$:

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



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

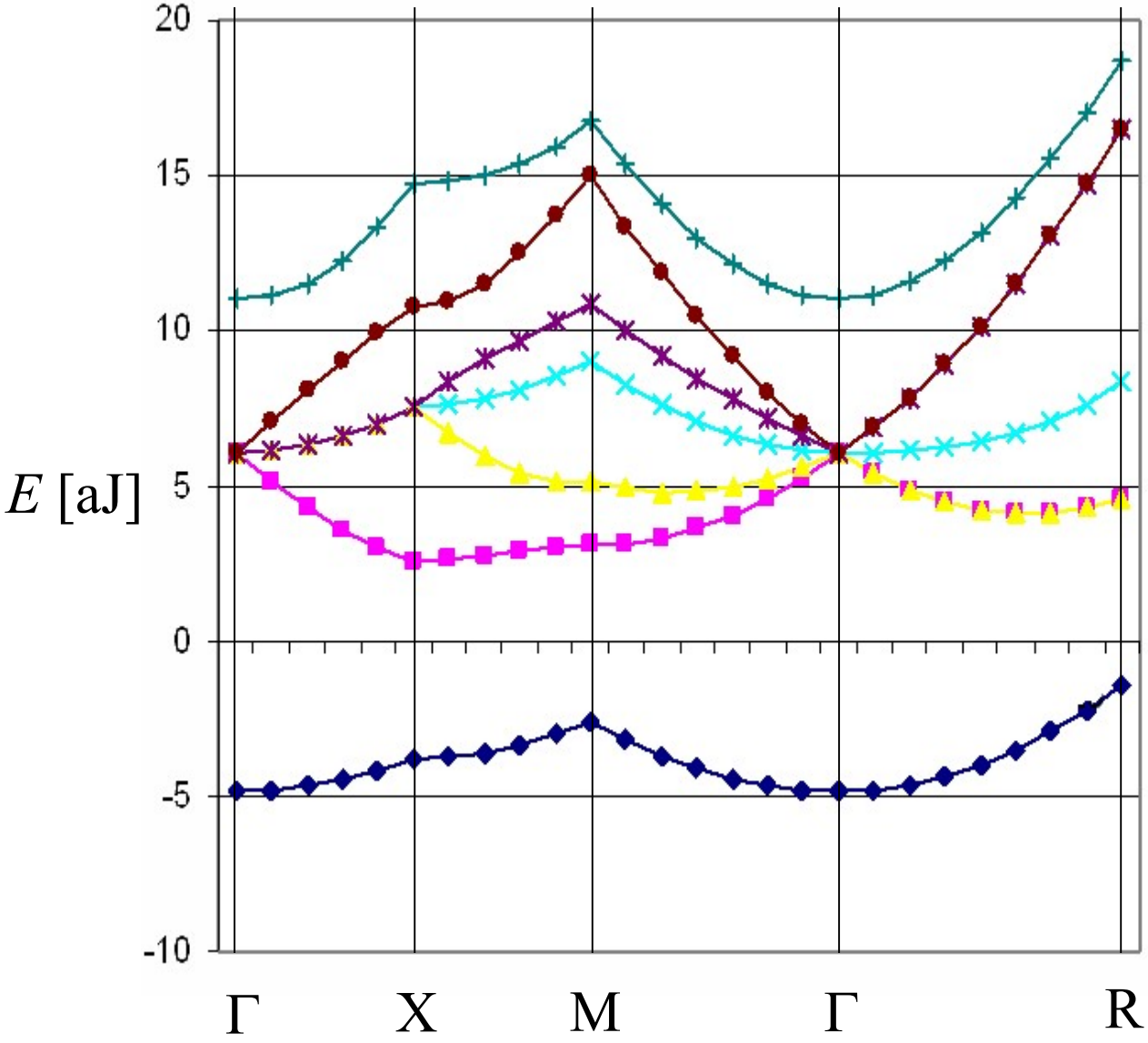
diagonal elements: $$\frac{\hbar^2}{2m}\left(\vec{k} - \vec{G}_i\right)^2$$

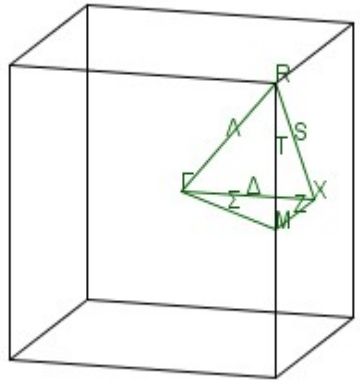
off-diagonal elements: $$\frac{-Ze^2}{V_{\text{unit cell}}\varepsilon_0 \left(\vec{G}_i - \vec{G}_j\right)^2}$$

Central equations - simple cubic

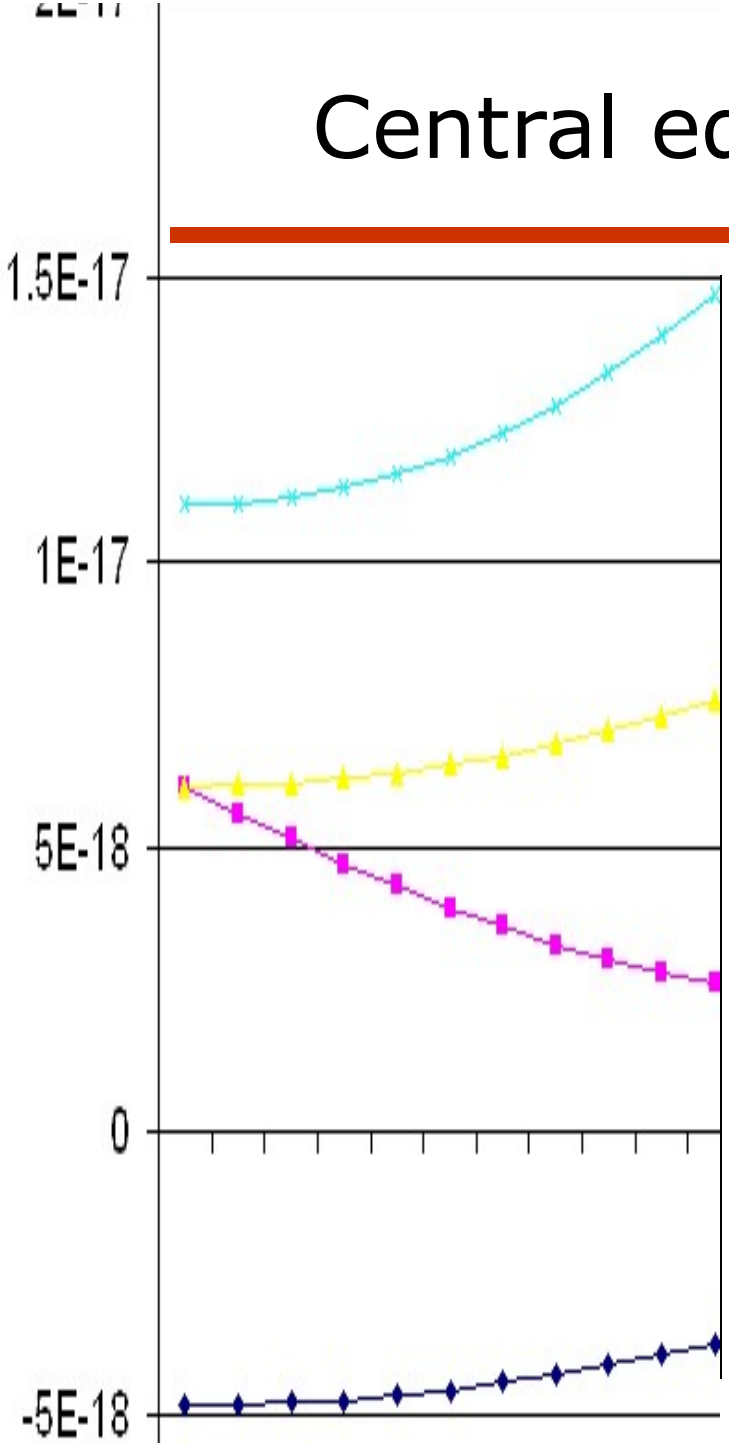
$$
\begin{pmatrix}
\frac{\hbar^2\left(\vec{k}+\frac{2\pi}{a}\hat{k}_z\right)^2}{2m} & \frac{-Ze^2a^2}{8V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{-Ze^2a^2}{8V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{-Ze^2a^2}{4V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{-Ze^2a^2}{8V_{\text{unit cell}}\varepsilon_0\pi^2}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

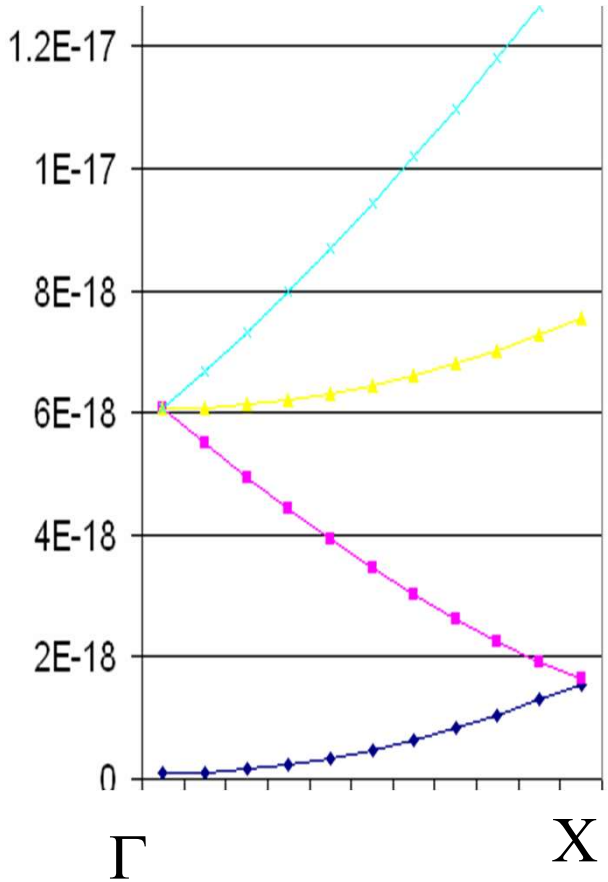


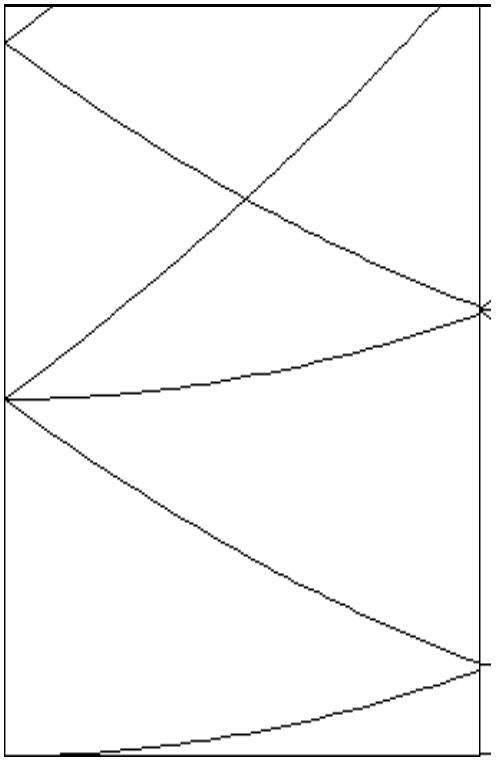


Central equations - simple cubic



empty lattice





Plane Wave Method

Download this Jupyter notebook

The plane wave method can be used to calculate the electronic band structures of materials. In this method, the Schrödinger equation is solved for the energy eigenstates of a single electron moving in a periodic potential. Since there is only one electron in the problem, electron-electron interactions are neglected except by possibly including the average positions of the other electrons in the periodic potential that the single electron sees. The ground state and some excited states for the single electron are determined for every $\vec{k}$ -vector in the first Brillouin zone. To determine the properties of the many electron system, the single electron states are filled starting with the lowest energy states and filling the electron states up to the Fermi energy. The Schrödinger equation for a single electron is,

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

Since the potential $U(\vec{r})$ and the wave function ψ are periodic functions, they can be written as Fourier series,

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

$$\psi(\vec{r}) = \sum_{\vec{k}} C_{\vec{k}} e^{i\vec{k}\cdot\vec{r}}.$$

The potential $U(\vec{r})$ has the periodicity of the lattice, so the Fourier series for it sums over the reciprocal lattice vectors $\vec{G}$. The wave function can be any function that satisfies the periodic boundary conditions of a box that contains many unit cells of the crystal. The wavevectors $\vec{k}$ satisfy the periodic boundary conditions of this box. Substituting this form for the potential and the wave function into the Schrödinger equation yields,

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

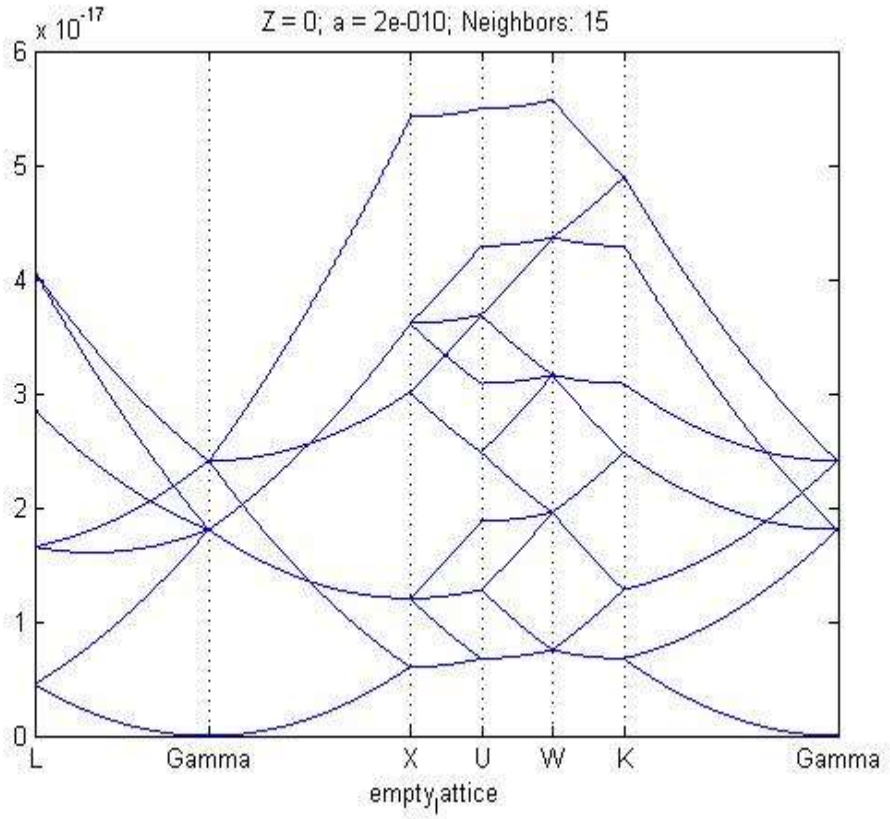
In the middle term with the double sum, the sum over $\vec{k}$ has been relabeled as a sum over $\vec{k}'$. It does not matter that the label has changed since the sum is over all of the states. Next we collect like terms. The exponential factors can be written as $e^{i\vec{k}\cdot\vec{r}} = \cos(\vec{k}\cdot\vec{r}) + i\sin(\vec{k}\cdot\vec{r})$. Only terms that have the same wavelength can be equal to each other so only the terms where $\vec{k} = \vec{G} + \vec{k}'$ can be equal to each other. This results in the condition,

$$\frac{\hbar^2 k^2}{2m} C_{\vec{k}} + \sum_{\vec{G}} U_{\vec{G}} C_{\vec{k}-\vec{G}} = E C_{\vec{k}}.$$

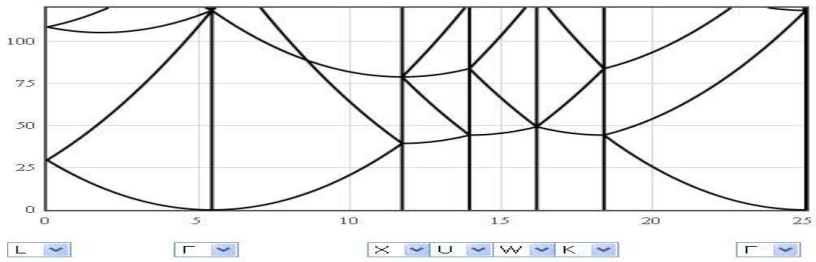
http://lampx.tugraz.at/~hadley/ss1/bands/planewave/Plane_Wave_fcc.html

Plane wave method

fcc Z= 0

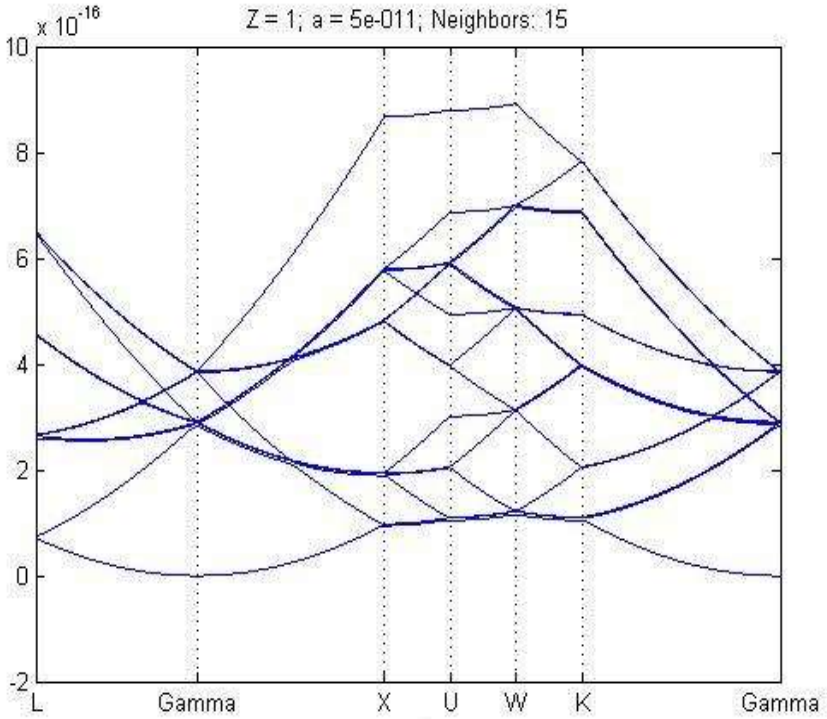


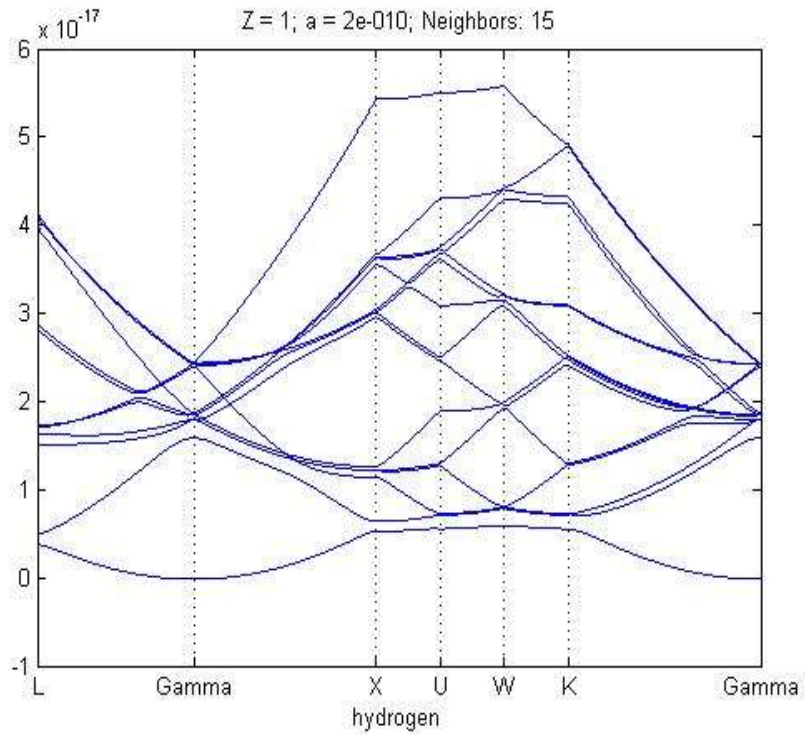
empty lattice



Plane wave method

fcc hydrogen





Approximate solution near the Bz boundary

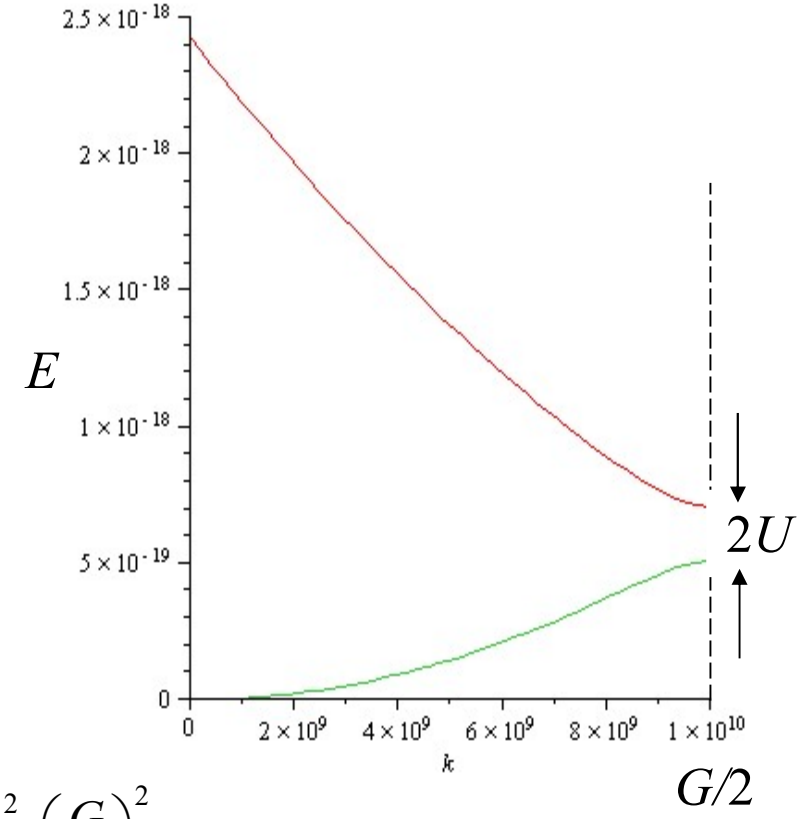
$$\left(\frac{\hbar^2 k^2}{2m} - E\right) C_k + \sum_G U_G C_{k-G} = 0$$

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 $k \sim G/2$

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



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

Review: Molecules

Start with the full Hamiltonian

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

Use the Born-Oppenheimer approximation

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

Neglect the electron-electron interactions. H_{elec} is then a sum of H_{MO}.

$$H_{MO} = \frac{-\hbar^2}{2m_e}\nabla_1^2 - \sum_A \frac{Z_A e^2}{4\pi\varepsilon_0 \left| r_1 - r_A \right|}$$

The molecular orbital Hamiltonian can be solved numerically or by the Linear Combinations of Atomic Orbitals (LCAO)

Linear combination of atomic orbitals

Guess that the solution to H_{mo} can be written as a linear combination of atomic orbitals.

$$\psi_{mo} = c_1\phi^H_{1s,A} + c_2\phi^H_{1s,B} + c_3\phi^H_{2s,A} + c_4\phi^H_{2s,B} + \cdots$$

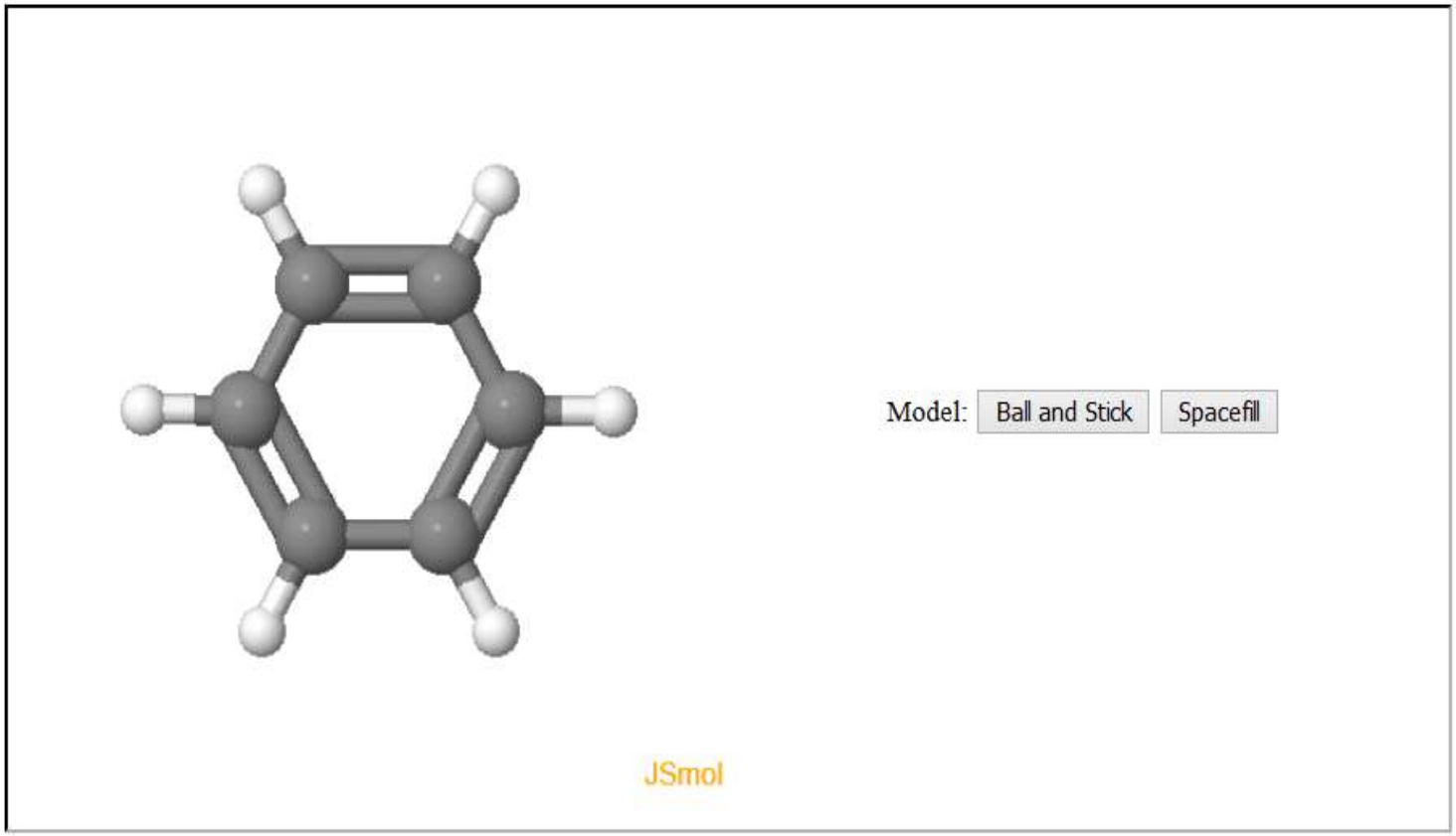
Construct the Hamiltonian matrix.

$$\begin{bmatrix} \langle \phi^H_{1s,A} | H_{mo} | \phi^H_{1s,A} \rangle & \langle \phi^H_{1s,A} | H_{mo} | \phi^H_{1s,B} \rangle \\ \langle \phi^H_{1s,B} | H_{mo} | \phi^H_{1s,A} \rangle & \langle \phi^H_{1s,B} | H_{mo} | \phi^H_{1s,B} \rangle \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = E \begin{bmatrix} \langle \phi^H_{1s,A} | \phi^H_{1s,A} \rangle & \langle \phi^H_{1s,A} | \phi^H_{1s,B} \rangle \\ \langle \phi^H_{1s,B} | \phi^H_{1s,A} \rangle & \langle \phi^H_{1s,B} | \phi^H_{1s,B} \rangle \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix}$$

$$S \approx \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Molecular orbitals of benzene

Benzene (C_6H_6) consists of 6 carbon atoms in a ring. A hydrogen atom is attached to each carbon atom. The carbon-carbon bond length is 1.40 Å and the carbon-hydrogen bond length is 1.10 Å.



$$\psi_{\mathrm{mo},j} = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} \exp\left(\frac{i2\pi nj}{N}\right) \phi_{2pz}^{C}(\vec{r} - \vec{r}_n) \qquad j = 1, 2, \cdots, N.$$

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.

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

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

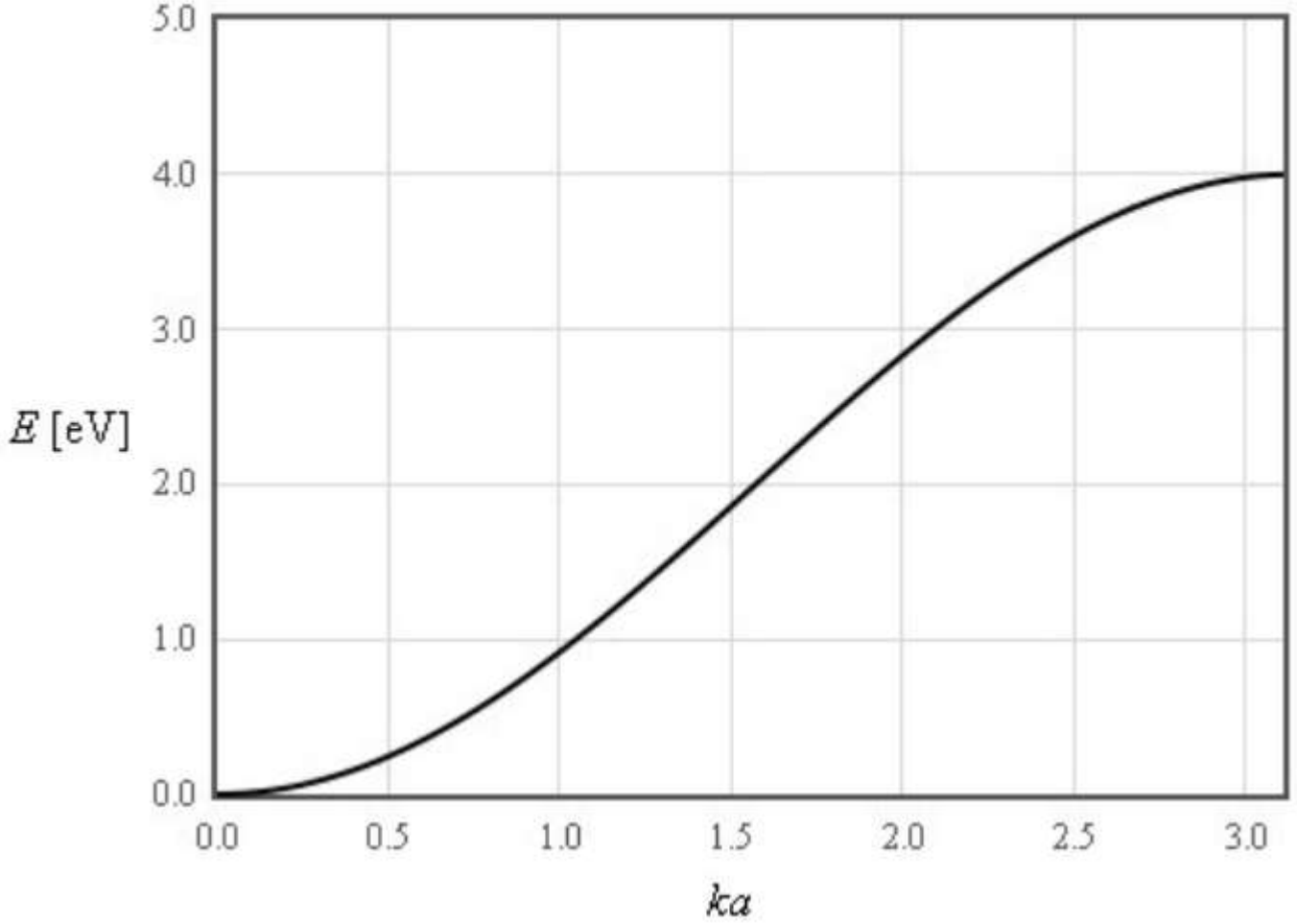
$$= E + \text{small terms}.$$

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

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

Tight binding: 1-D chain

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



Tight binding

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.

$$T_{pqs}\psi_k = \exp\left(i\left(p\vec{k}\cdot\vec{a}_1 + q\vec{k}\cdot\vec{a}_2 + s\vec{k}\cdot\vec{a}_3\right)\right)\psi_k$$

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

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

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

$$\varepsilon = \langle \phi_a(\vec{r}) | H_{MO} | \phi_a(\vec{r}) \rangle$$

On-site energy

$$t = -\langle \phi_a(\vec{r}) | H_{MO} | \phi_a(\vec{r} - \vec{\rho}_m) \rangle$$

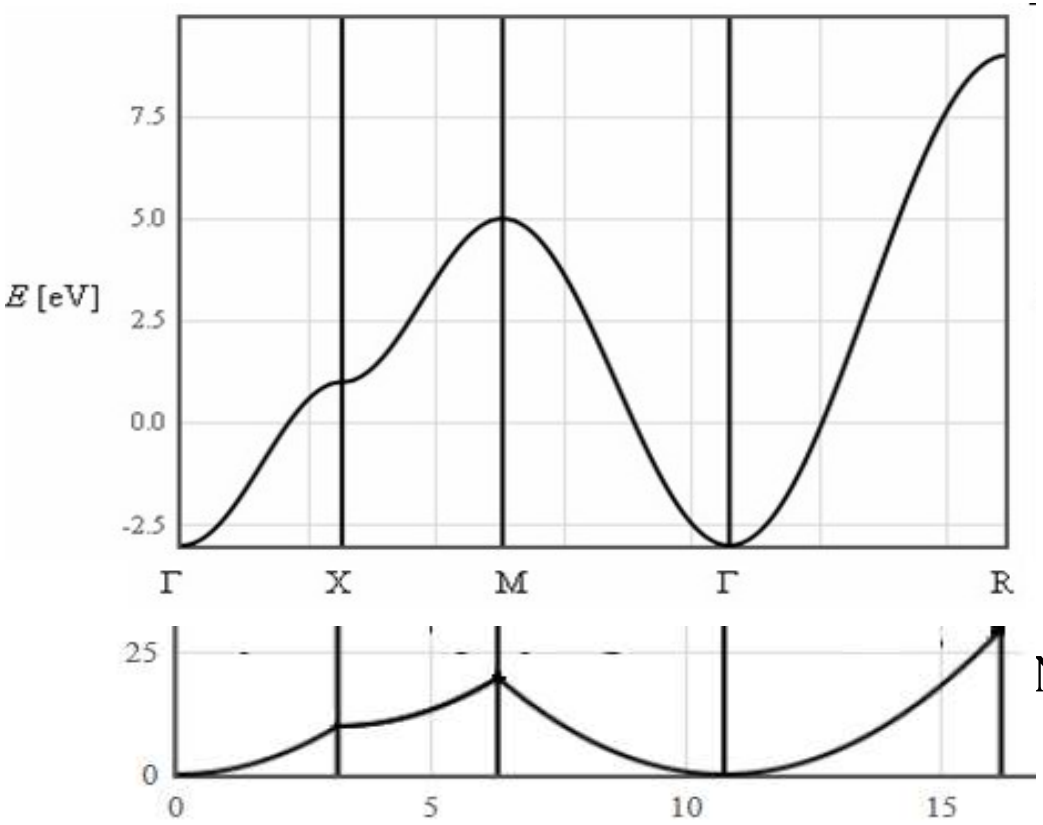
Overlap integral

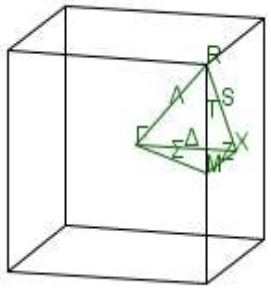
Tight binding, simple cubic

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

$$E = \varepsilon - t\left(e^{ik_x a} + e^{-ik_x a} + e^{ik_y a} + e^{-ik_y a} + e^{ik_z a} + e^{-ik_z a}\right)$$

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

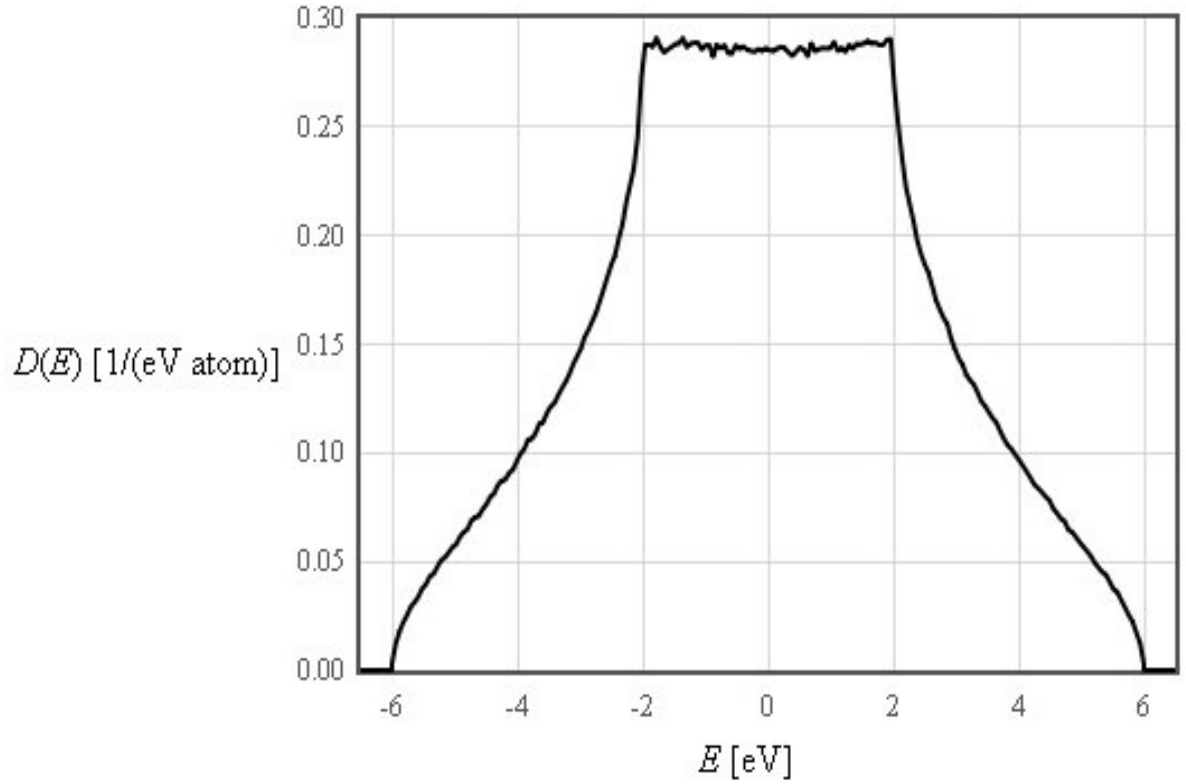




Effective mass $m^* = \dfrac{\hbar^2}{\dfrac{d^2E}{dk^2}} = \dfrac{\hbar^2}{2ta^2}$

Narrow bands → high effective mass

Density of states (simple cubic)



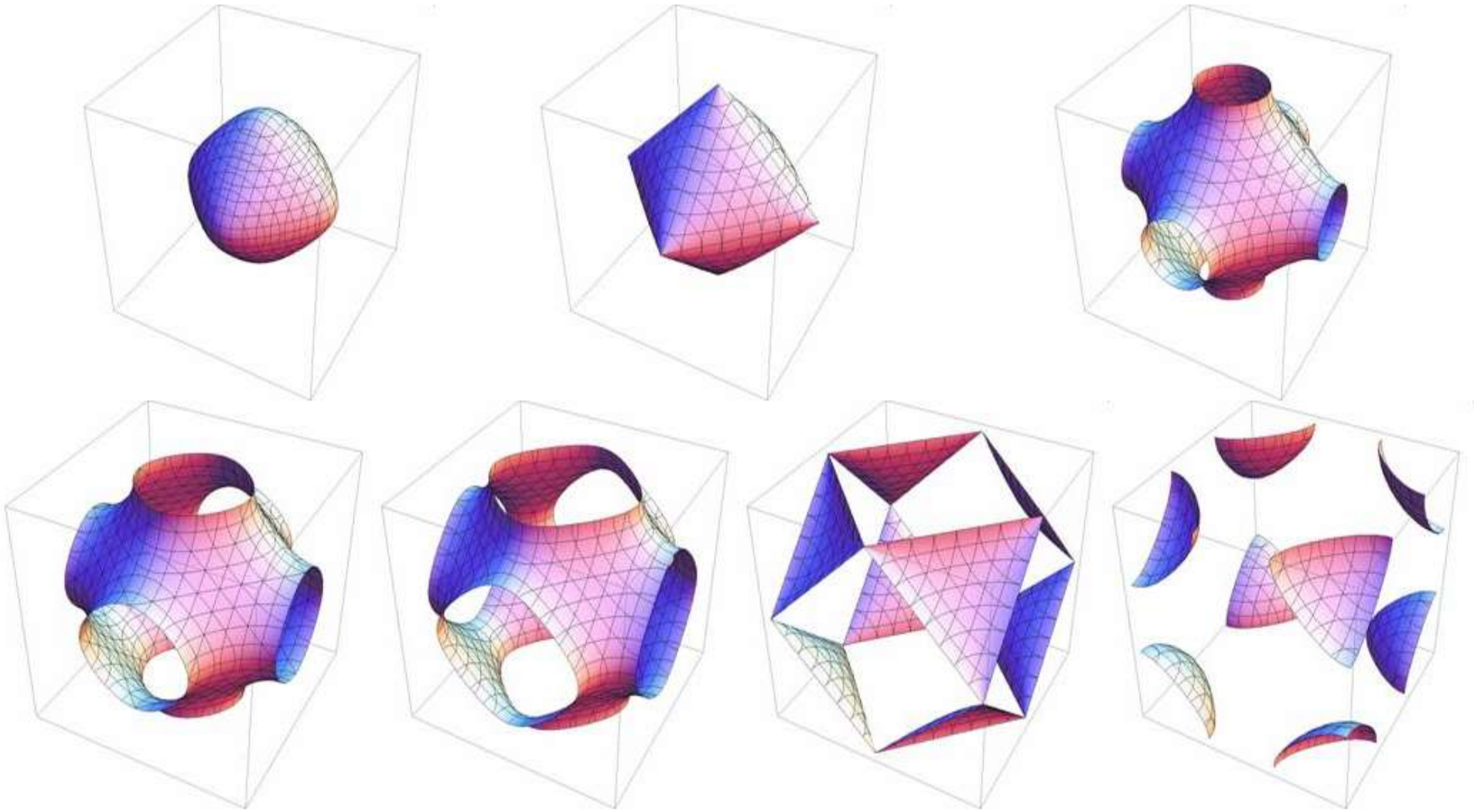
Calculate the energy for every allowed k in the Brillouin zone

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

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

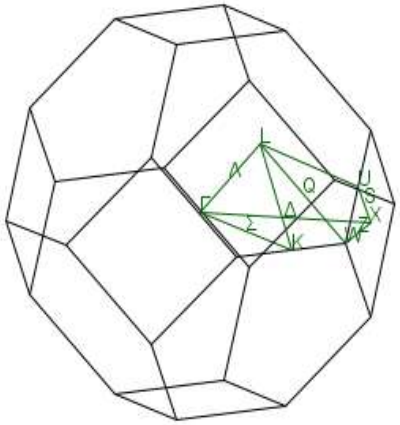
Tight binding, simple cubic

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



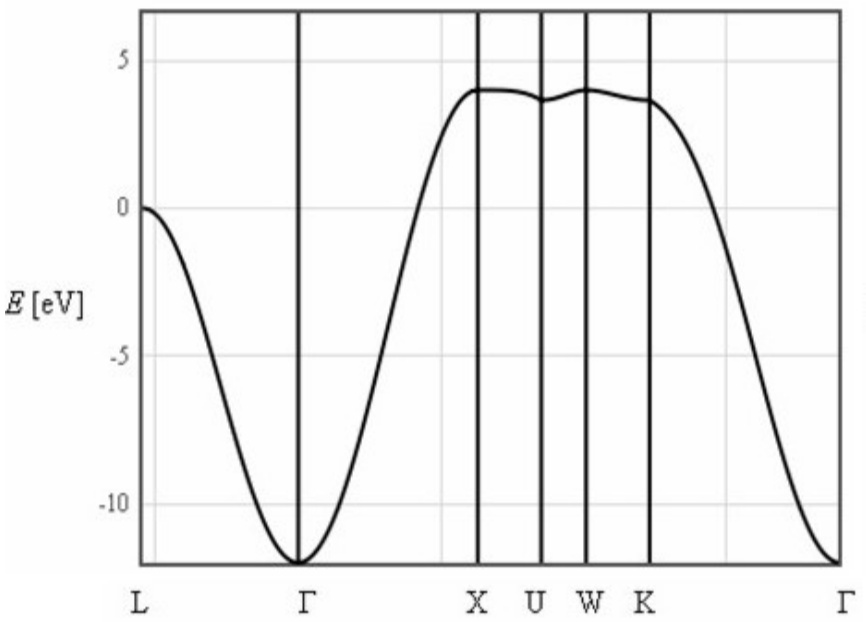
Christian Gruber, 2008

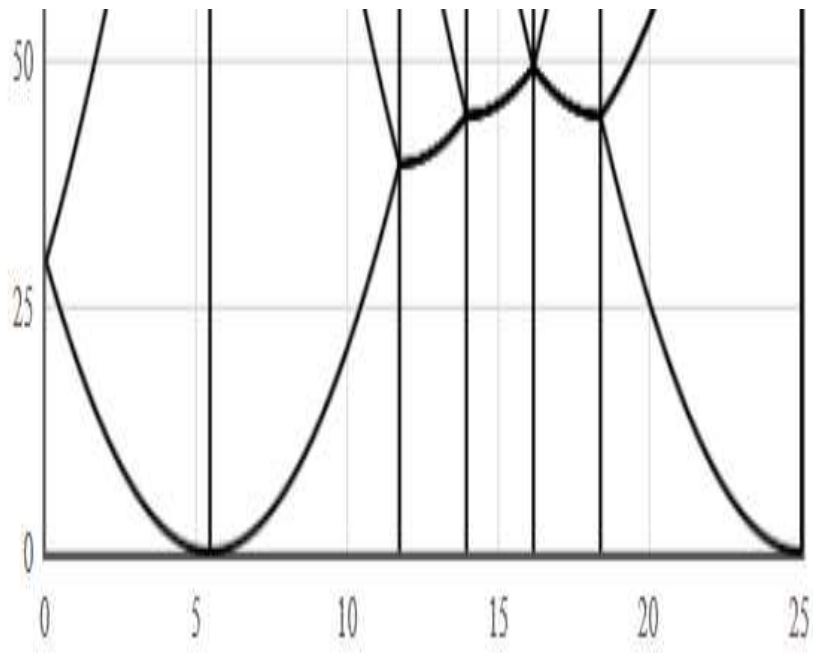
Tight binding, fcc



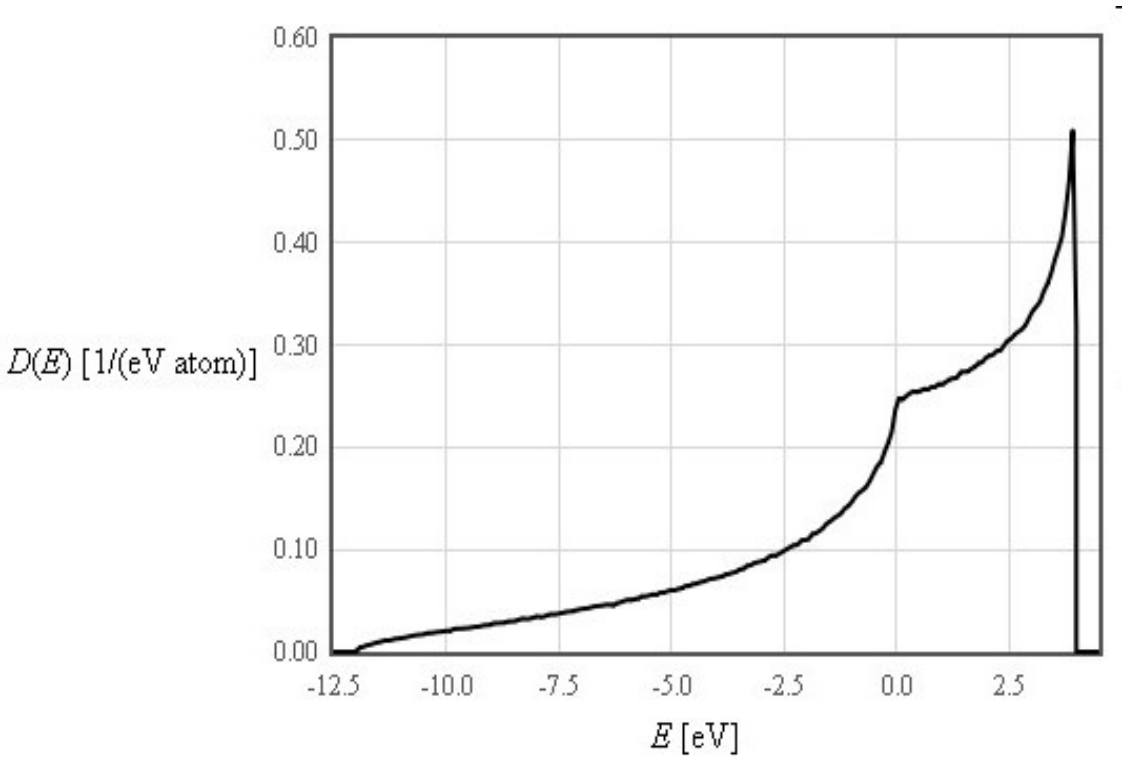
$$E = \varepsilon - t\sum_{lmn} e^{i\vec{k}\cdot\vec{\rho}_{lmn}}$$

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





Density of states (fcc)

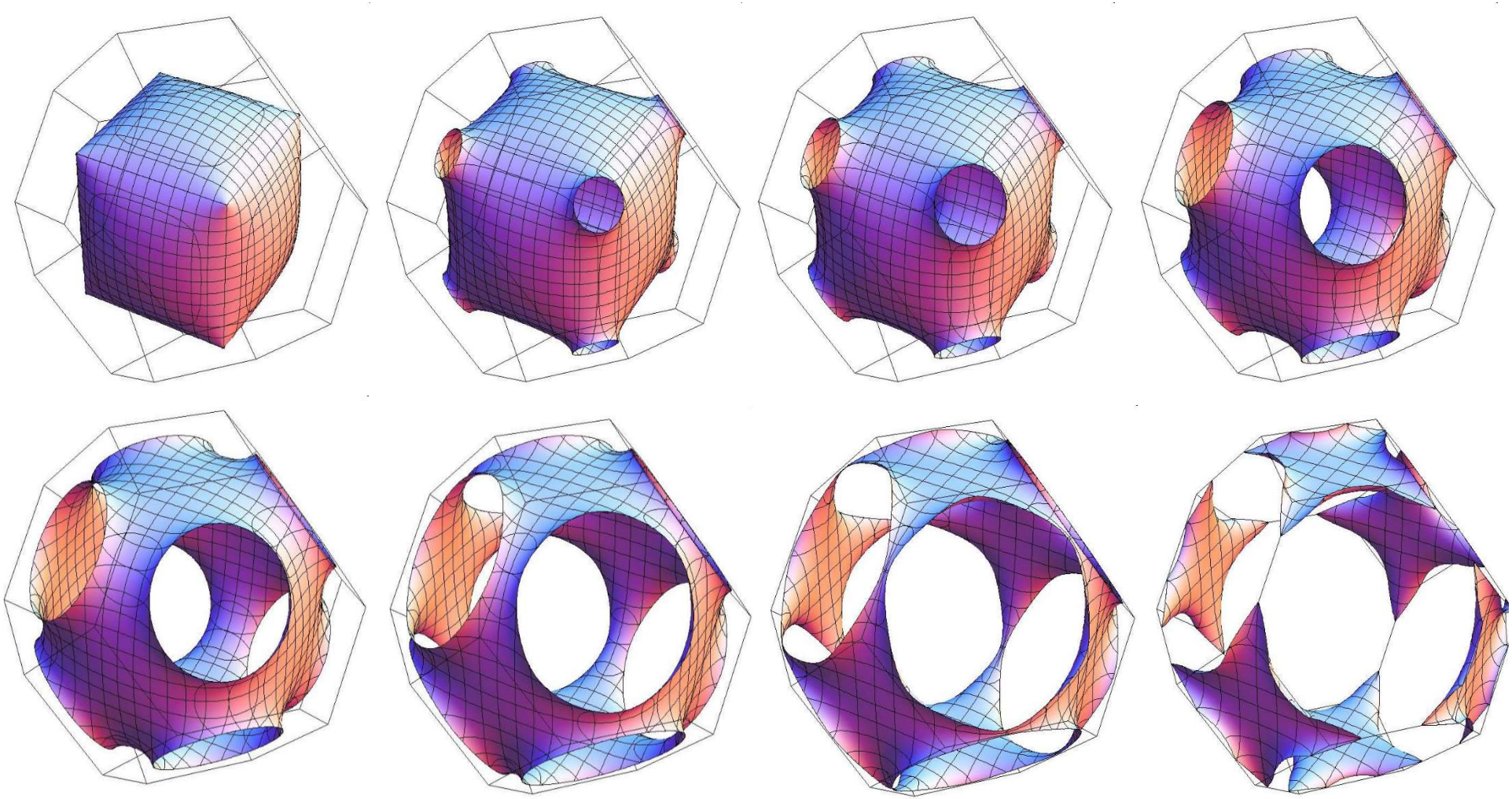


Calculate the energy for every allowed k in the Brillouin zone

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

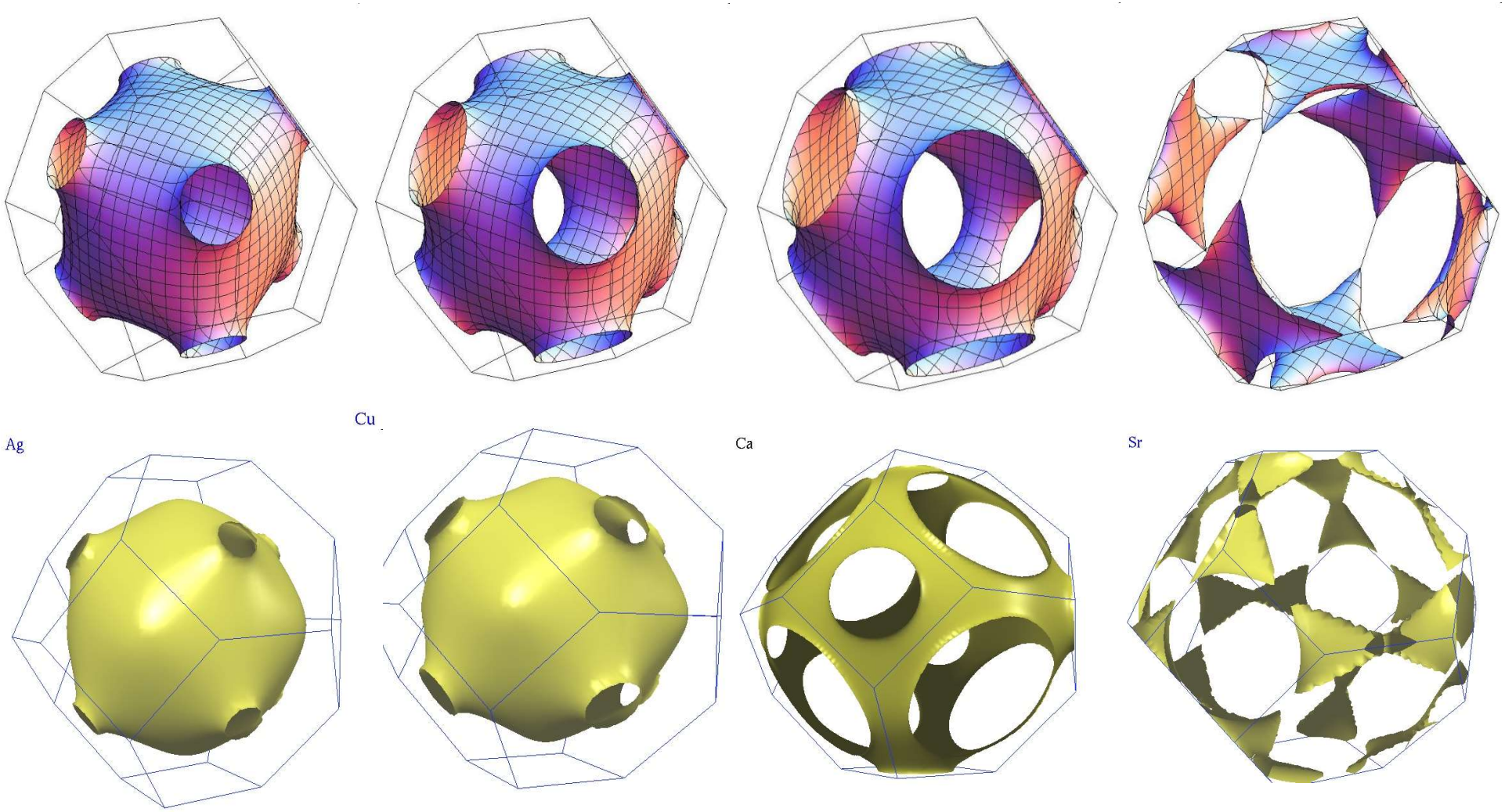
http://lamp.tu-graz.ac.at/~hadley/ss1/bands/tbtable/tbtable.html

Tight binding, fcc



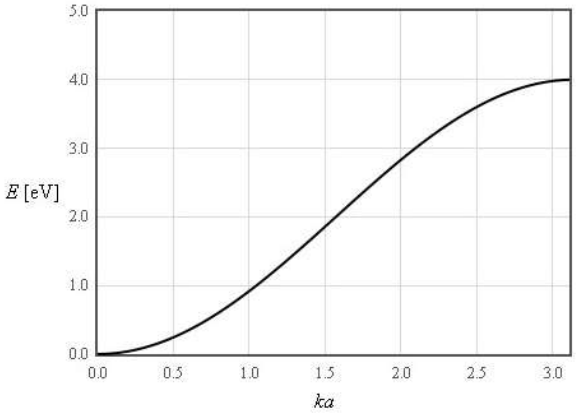
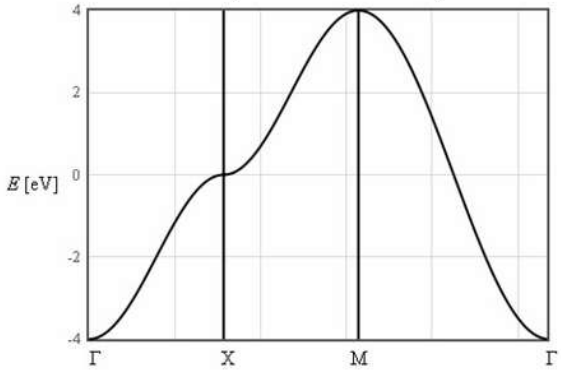
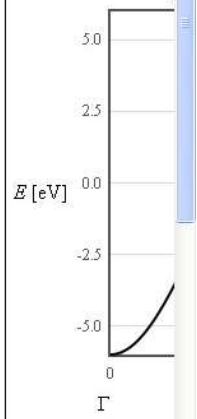
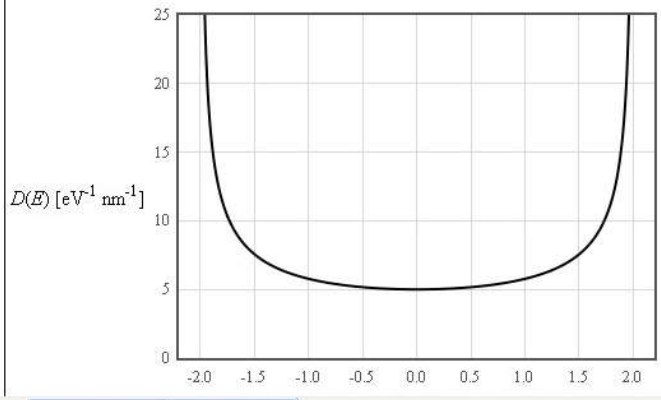
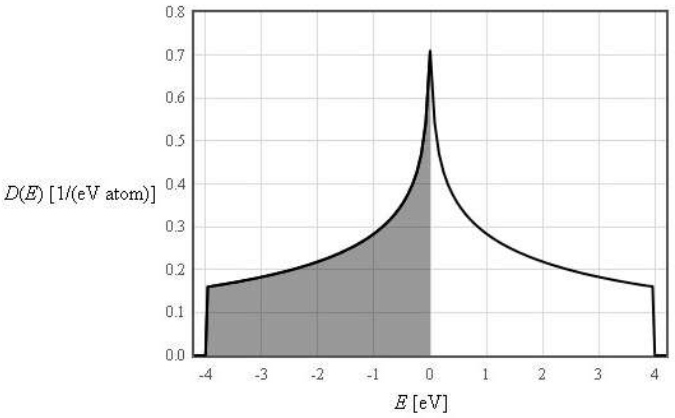
Christian Gruber, 2008

Tight binding, fcc

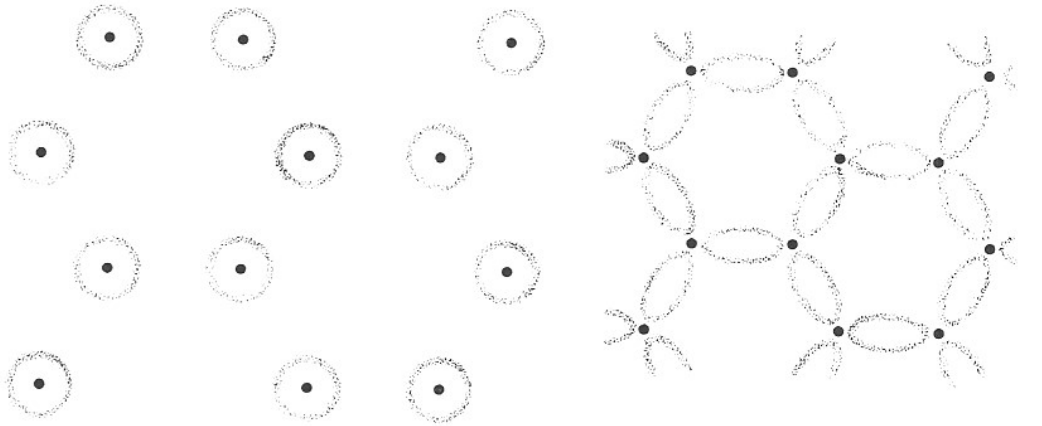


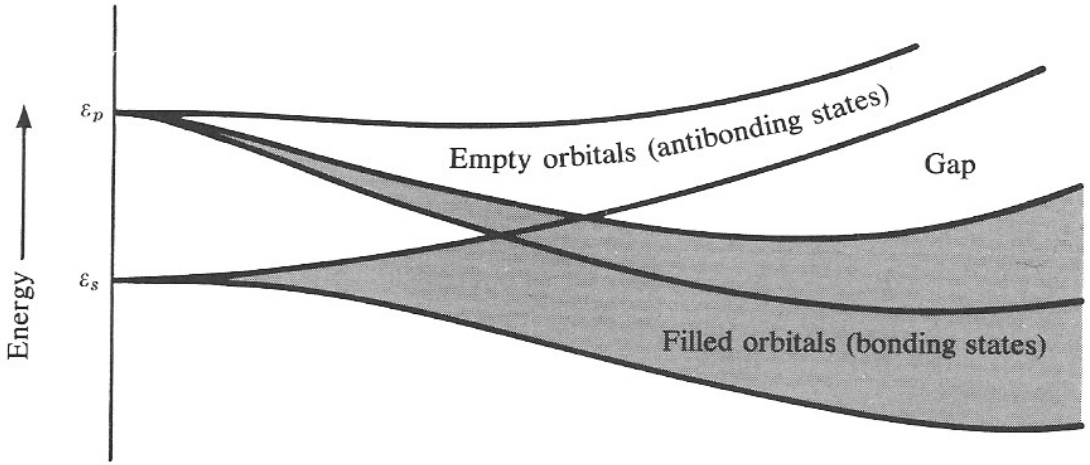
http://www.phys.ufl.edu/fermisurface/

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

Tight binding





Harrison, Electronic Structure, Freeman 1980

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.

There are N translational symmetries.

Each k state can hold 2 electrons (spin).

There are $2N$ states per Brillouin zone.

2N electron states/band

N primitive unit cells = k-states in 1st Bz

Tight-binding: p atomic orbitals/primitive unit cell

p bands each of which can hold $2N$ electrons