Plane wave method
Tight binding

Bloch Theorem

Bloch form $\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} u_{\vec{k}}(\vec{r})$

Eigenfunction solutions of the Schrödinger equation have Bloch form.

k is a wave vector in the 1st Brillouin zone

$u_{\vec{k}}(\vec{r})$ is a periodic function

Plane wave method

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

The potential is periodic $$U(\vec{r}) = \sum_{\vec{G}} U_{\vec{G}} e^{i\vec{G}\cdot\vec{r}}$$

Bloch form $$\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} \sum_{\vec{G}'} C_{\vec{G}'} e^{i\vec{G}'\cdot\vec{r}}$$

$$\sum_{\vec{G}} C_{\vec{G}} e^{i\vec{G}\cdot\vec{r}} = \sum_{\vec{G}'} C_{\vec{G}'} e^{i\vec{G}'\cdot\vec{r}}$$

We can relabel the reciprocal lattice vectors since we sum over them.

Plane wave method

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

Only the terms with the same wavelength can be equal to each other.

$$\vec{G}'' = \vec{G}' - \vec{G}$$

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

There is one equation for each $\vec{G}'$ vector.

Plane wave method

Central equations: $$\frac{\hbar^2(\vec{k}+\vec{G}')^2}{2m}C_{\vec{G}'}+\sum_{\vec{G}}U_{\vec{G}}C_{\vec{G}'-\vec{G}}=EC_{\vec{G}'}$$

$$\frac{\hbar^2(k-G_0)^2}{2m}C_{-G_0}+(\cdots+U_{-2G_0}C_{G_0}+U_{-G_0}C_0+U_0C_{-G_0}+\cdots)=EC_{-G_0}.$$

$$\frac{\hbar^2k^2}{2m}C_0+(\cdots+U_{-G_0}C_{G_0}+U_0C_0+U_{G_0}C_{-G_0}+\cdots)=EC_0.$$

$$\frac{\hbar^2(k+G_0)^2}{2m}C_{G_0}+(\cdots+U_0C_{G_0}+U_{G_0}C_0+U_{2G_0}C_{-G_0}+\cdots)=EC_{G_0}.$$

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

Central equations - one dimension

$$\frac{\hbar^2(\vec{k}+\vec{G}')^2}{2m}C_{\vec{G}'}+\sum_{\vec{G}}U_{\vec{G}}C_{\vec{G}'-\vec{G}}=EC_{\vec{G}'}$$

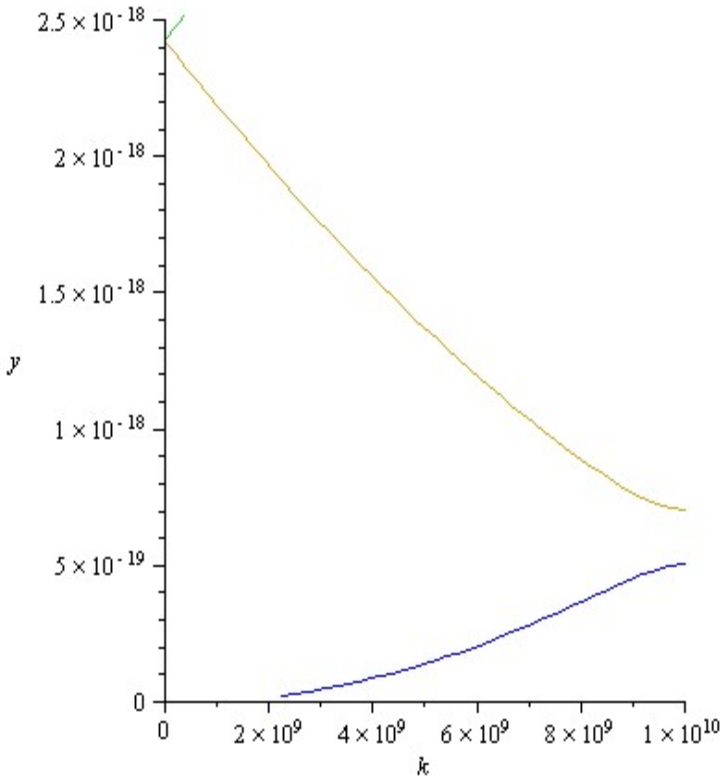
$$\begin{bmatrix}
\ddots & & & & & & \\
\frac{\hbar^2(k-2G_0)^2}{2m}+U_0-E & U_{-G_0} & U_{-2G_0} & U_{-3G_0} & U_{-4G_0} & U_{-5G_0} \\
U_{G_0} & \frac{\hbar^2(k-G_0)^2}{2m}+U_0-E & U_{-G_0} & U_{-2G_0} & U_{-3G_0} & U_{-4G_0} \\
U_{2G_0} & U_{G_0} & \frac{\hbar^2k^2}{2m}+U_0-E & U_{-G_0} & U_{-2G_0} & U_{-3G_0} \\
U_{3G_0} & U_{2G_0} & U_{G_0} & \frac{\hbar^2(k+G_0)^2}{2m}+U_0-E & U_{-G_0} & U_{-2G_0} \\
U_{4G_0} & U_{3G_0} & U_{2G_0} & U_{G_0} & \frac{\hbar^2(k+2G_0)^2}{2m}+U_0-E & U_{G_0} \\
 & & & & & \ddots
\end{bmatrix}
\begin{bmatrix}
\vdots \\ C_{-2G_0} \\ C_{-G_0} \\ C_0 \\ C_{G_0} \\ C_{2G_0} \\ \vdots
\end{bmatrix}=0$$

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

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

Molecular orbital Hamiltonian

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

Central equations:

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

diagonal elements:

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

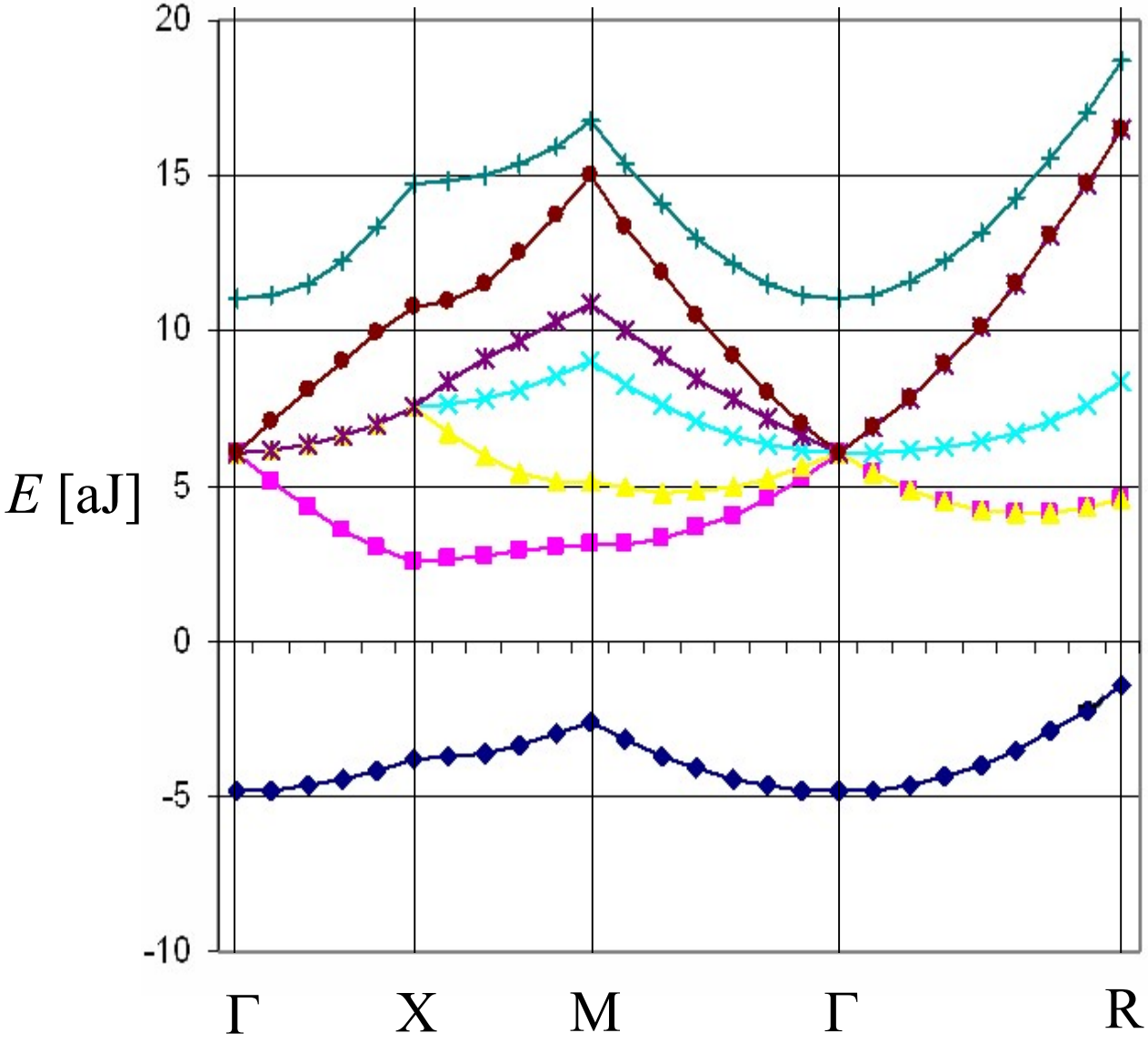
off-diagonal elements:

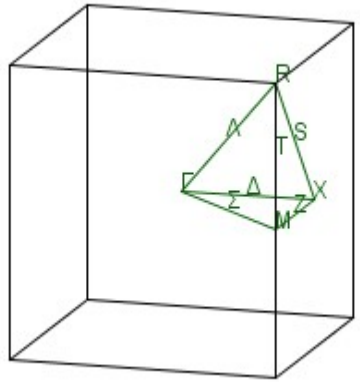
$$\frac{-Ze^2}{V_{\text{unit cell}}\varepsilon_0\left(\vec{G}_i-\vec{G}_j\right)^2}$$

Central equations - simple cubic

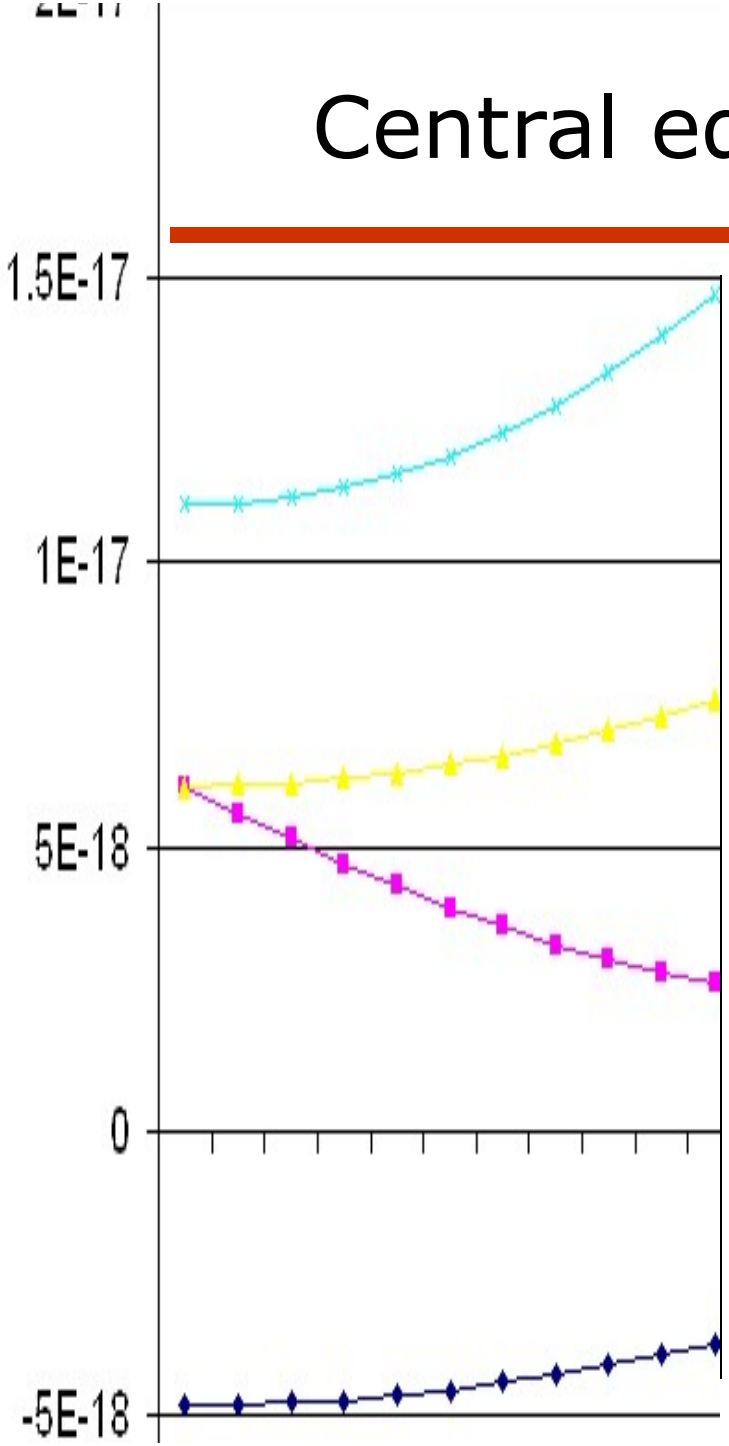
$$
\begin{pmatrix}
\frac{\hbar^2\left(\vec{k}+\frac{2\pi}{a}\hat{k}_z\right)^2}{2m} & \frac{-Ze^2a^2}{8V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{-Ze^2a^2}{8V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{-Ze^2a^2}{4V_{\text{unit cell}}\varepsilon_0\pi^2} & \frac{-Ze^2a^2}{8V_{\text{unit cell}}\varepsilon_0\pi^2}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

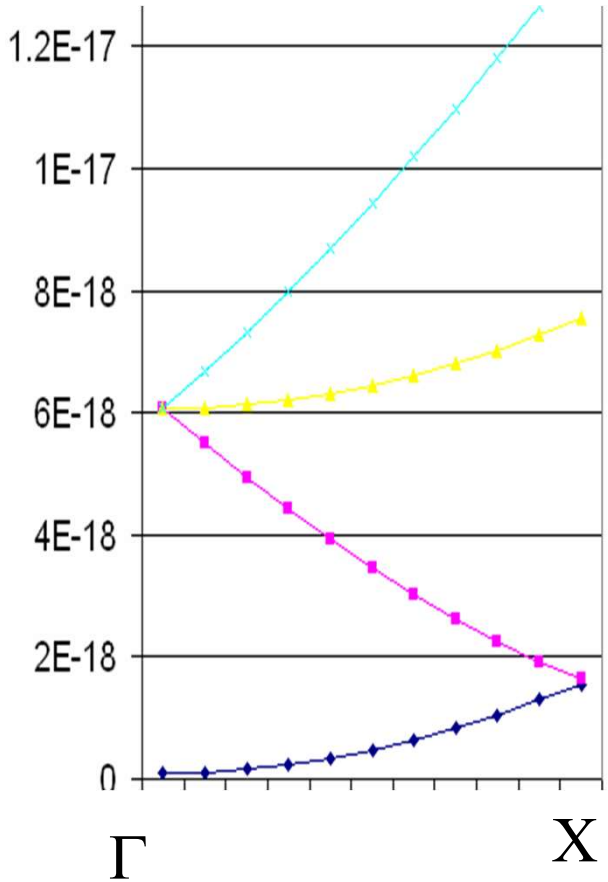


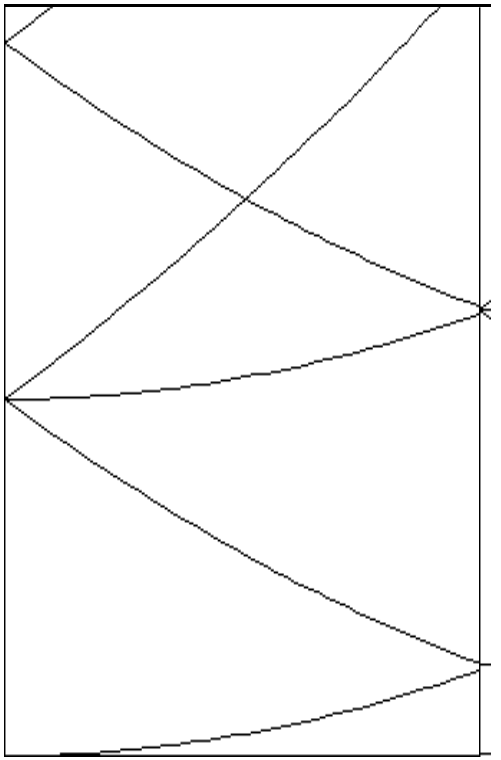


Central equations - simple cubic



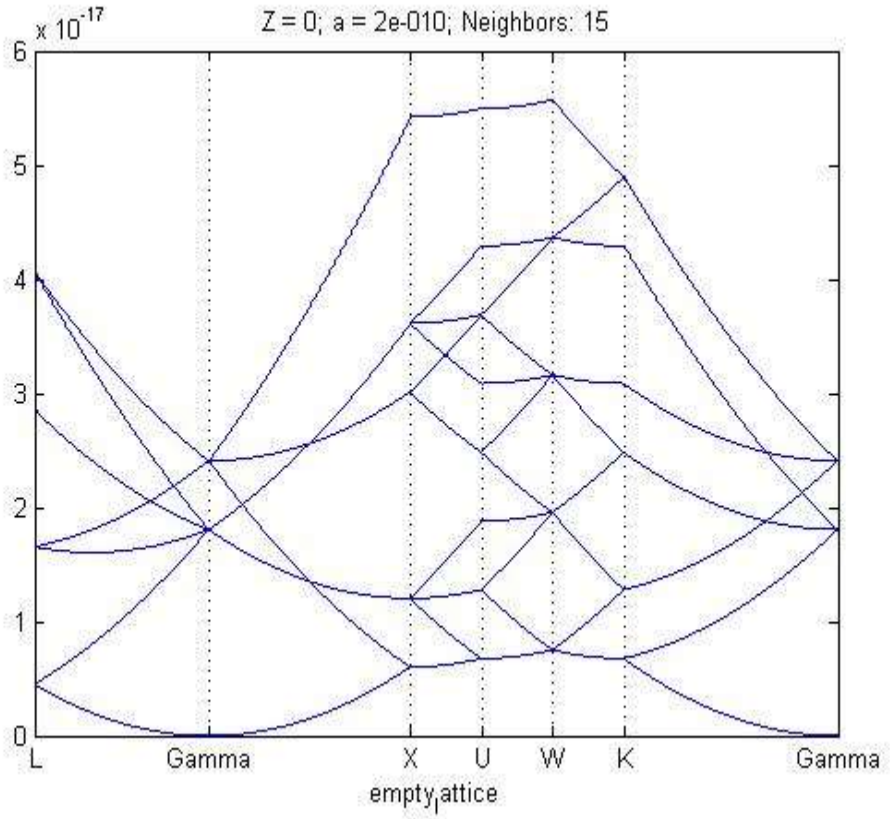
empty lattice



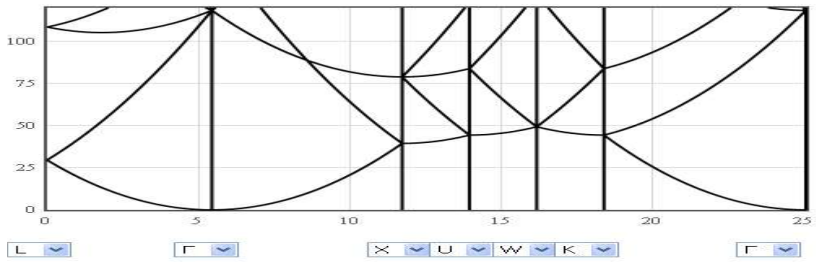


Plane wave method

fcc Z= 0

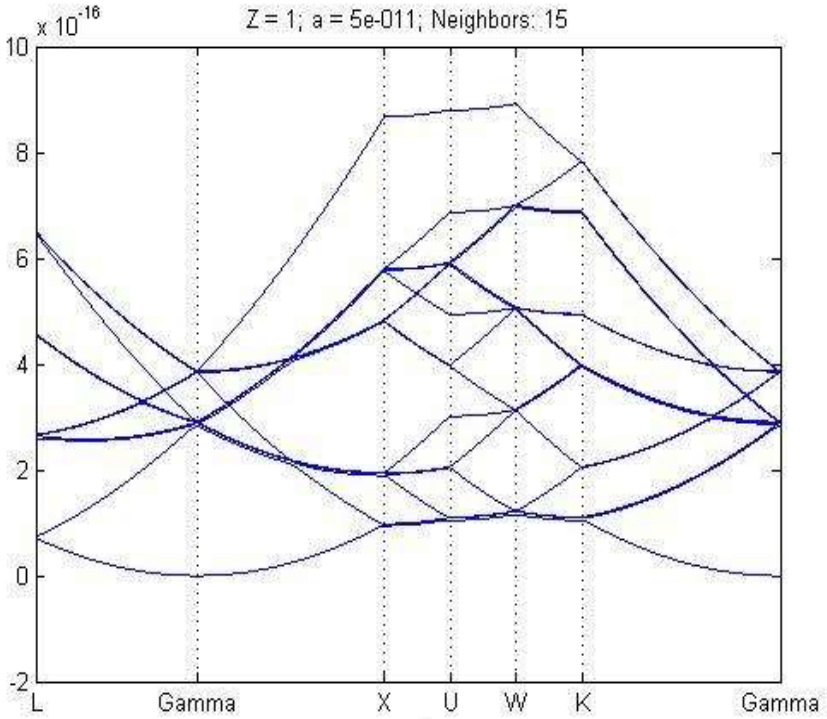


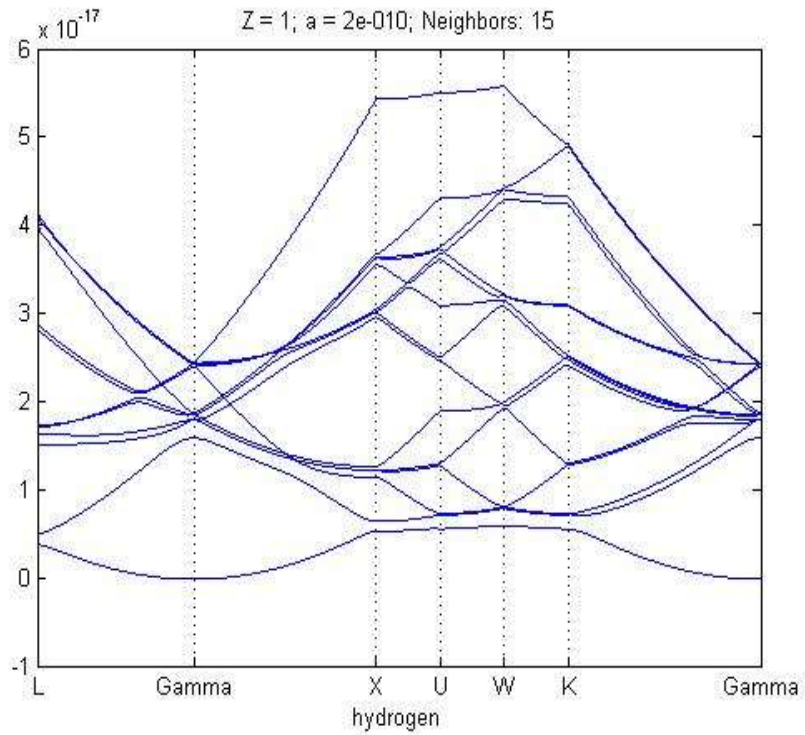
empty lattice



Plane wave method

fcc hydrogen





Approximate solution near the Bz boundary

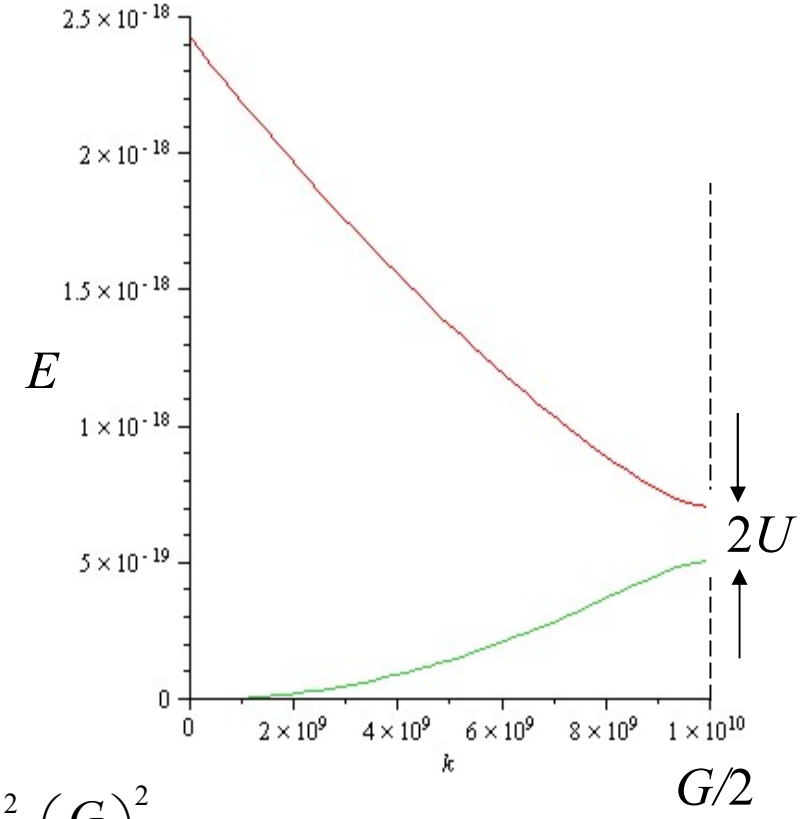
$$\frac{\hbar^2(\vec{k}+\vec{G}')^2}{2m}C_{\vec{G}'} + \sum_{\vec{G}} U_{\vec{G}} C_{\vec{G}'-\vec{G}} = EC_{\vec{G}'}$$

For just 2 terms

$$\begin{bmatrix} \frac{\hbar^2 k^2}{2m} - E & U \\ U & \frac{\hbar^2 (k-G)^2}{2m} - E \end{bmatrix} \begin{bmatrix} C_0 \\ C_{-G} \end{bmatrix} = 0$$

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

$$\begin{bmatrix} \frac{\hbar^2}{2m}\left(\frac{G}{2}\right)^2 - E & U \\ U & \frac{\hbar^2}{2m}\left(\frac{G}{2}\right)^2 - E \end{bmatrix} \begin{bmatrix} C_0 \\ C_{-G} \end{bmatrix} = 0$$



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

Tight binding
(Linear combination of atomic orbitals)

Apply the method of the Linear Combination of Atomic Orbitals to a molecule with periodic boundary conditions (like benzene).

Periodic function

$$\psi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{N}} \sum_{h,j,l} e^{i\left(h\vec{k}\cdot\vec{a}_1 + j\vec{k}\cdot\vec{a}_2 + l\vec{k}\cdot\vec{a}_3\right)} \sum_{a} \sum_{ao} c_{ao,a} \phi_{ao}^{Z_a}\left(\vec{r} - \vec{r}_a\right)$$

Sum over unit cell

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.

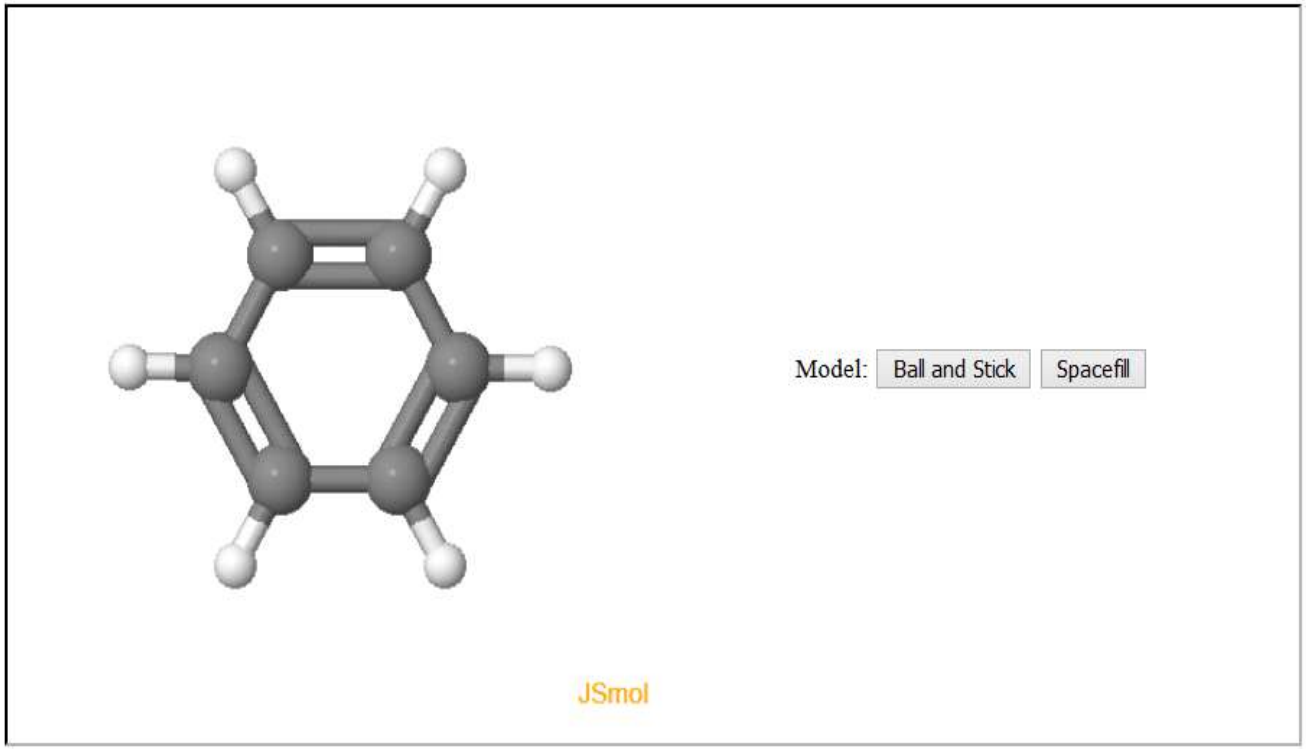
$$\psi_{mo} = c_1\phi^H_{1s,A} + c_2\phi^H_{1s,B} + c_3\phi^H_{2s,A} + c_4\phi^H_{2s,B} + \cdots$$

Construct the Hamiltonian matrix.

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

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.

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

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

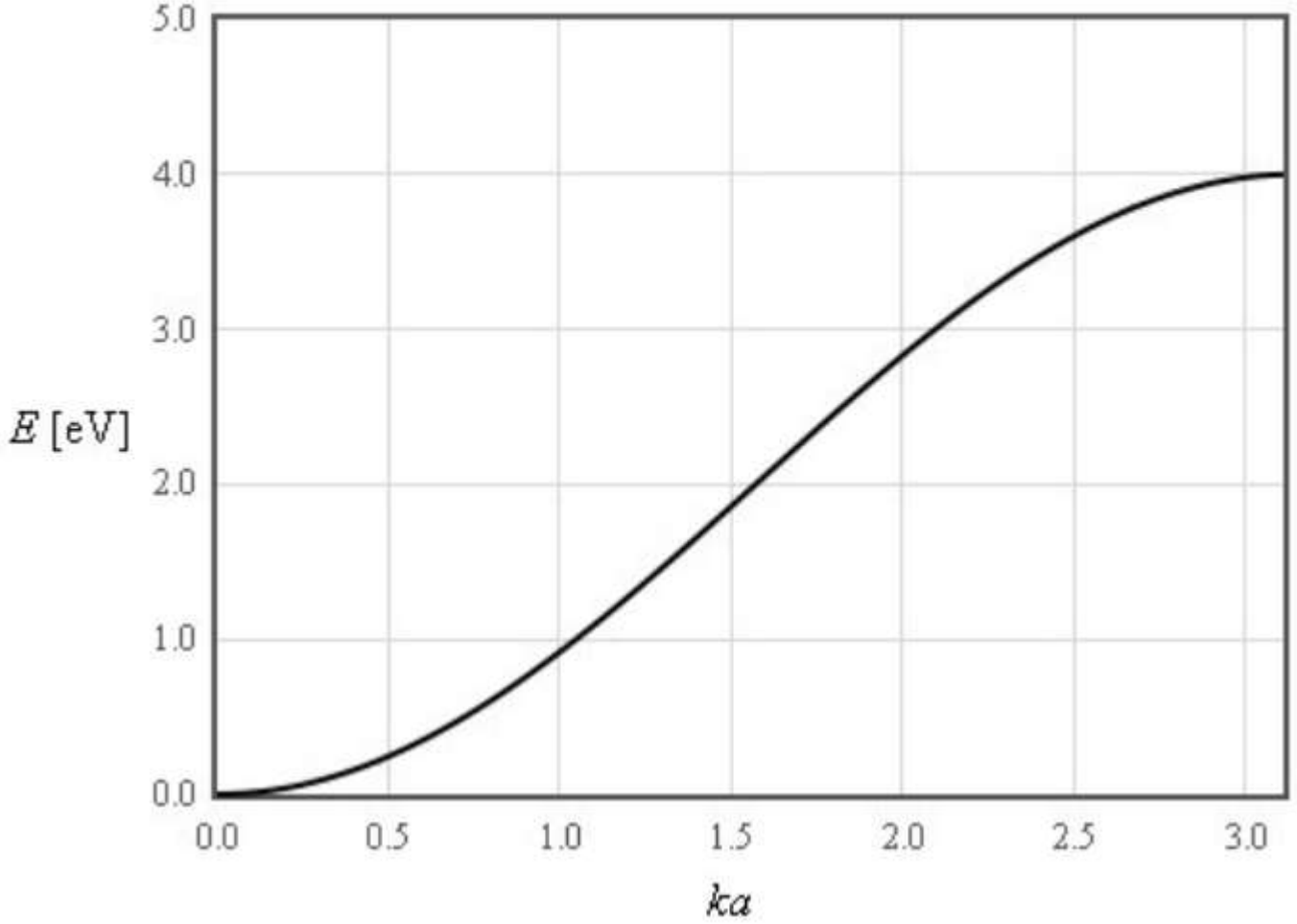
$$= E + \text{small terms}.$$

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

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

Tight binding: 1-D chain

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



Tight binding: 2 atoms, 1-D chain

$$\psi_k(x) = \frac{1}{\sqrt{L}} \sum_n e^{inka} \left(c_1 \phi_1(x - na) + c_2 \phi_2(x - na) \right)$$

$$\langle \phi_1 | \hat{H} | \psi_k \rangle = E \langle \phi_1 | \psi_k \rangle,$$
$$\langle \phi_2 | \hat{H} | \psi_k \rangle = E \langle \phi_2 | \psi_k \rangle.$$

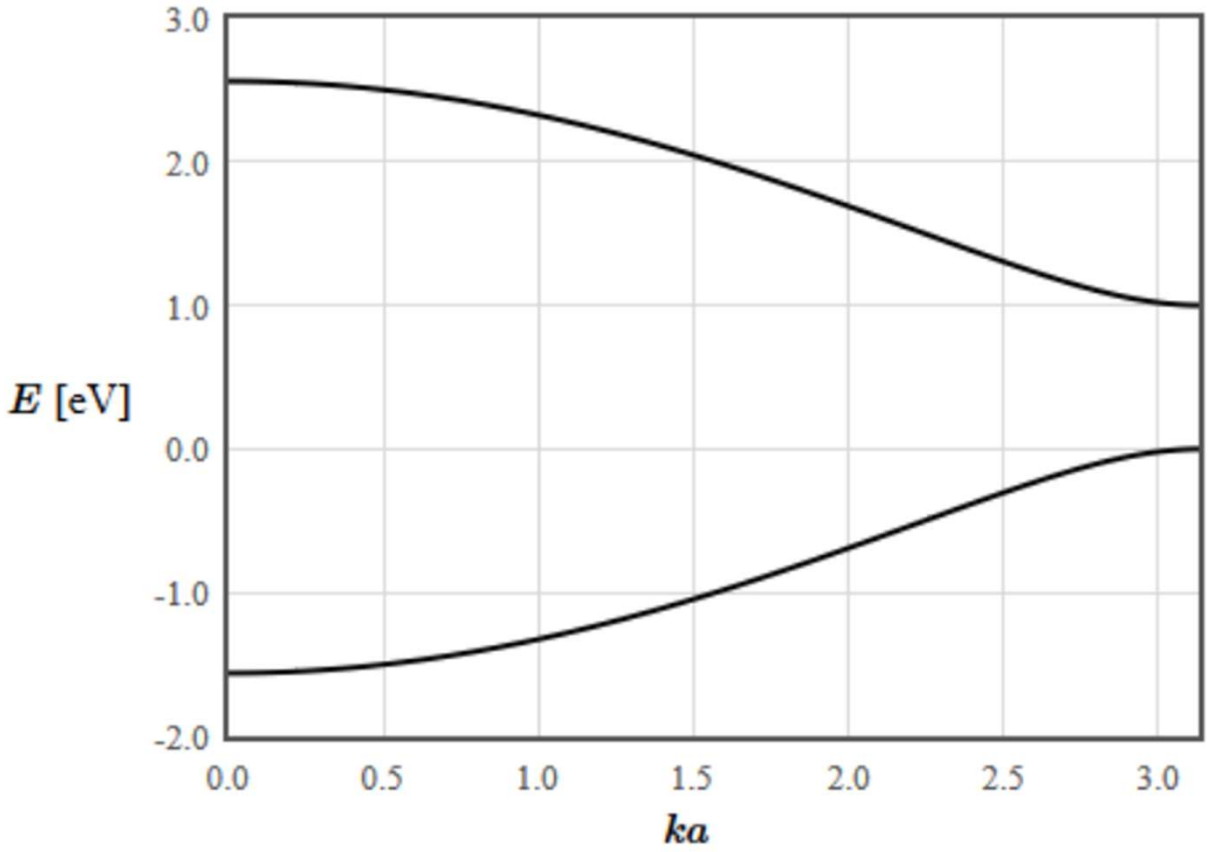
$$\epsilon_1 = \langle \phi_1(x) | \hat{H} | \phi_1(x) \rangle, \epsilon_2 = \langle \phi_2(x) | \hat{H} | \phi_2(x) \rangle$$

$$t = -\langle \phi_1(x) | \hat{H} | \phi_2(x) \rangle = -\langle \phi_2(x - a) | \hat{H} | \phi_1(x) \rangle$$

$$\begin{bmatrix} \epsilon_1 - E & -t\left(1 + e^{-ika}\right) \\ -t\left(1 + e^{ika}\right) & \epsilon_2 - E \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = 0.$$

Tight binding: 2 atoms, 1-D chain

$$E = \frac{(\epsilon_1 + \epsilon_2) \pm \sqrt{(\epsilon_1 - \epsilon_2)^2 + 8t^2(1 + \cos(ka))}}{2}.$$



2 orbitals → 2 bands

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

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

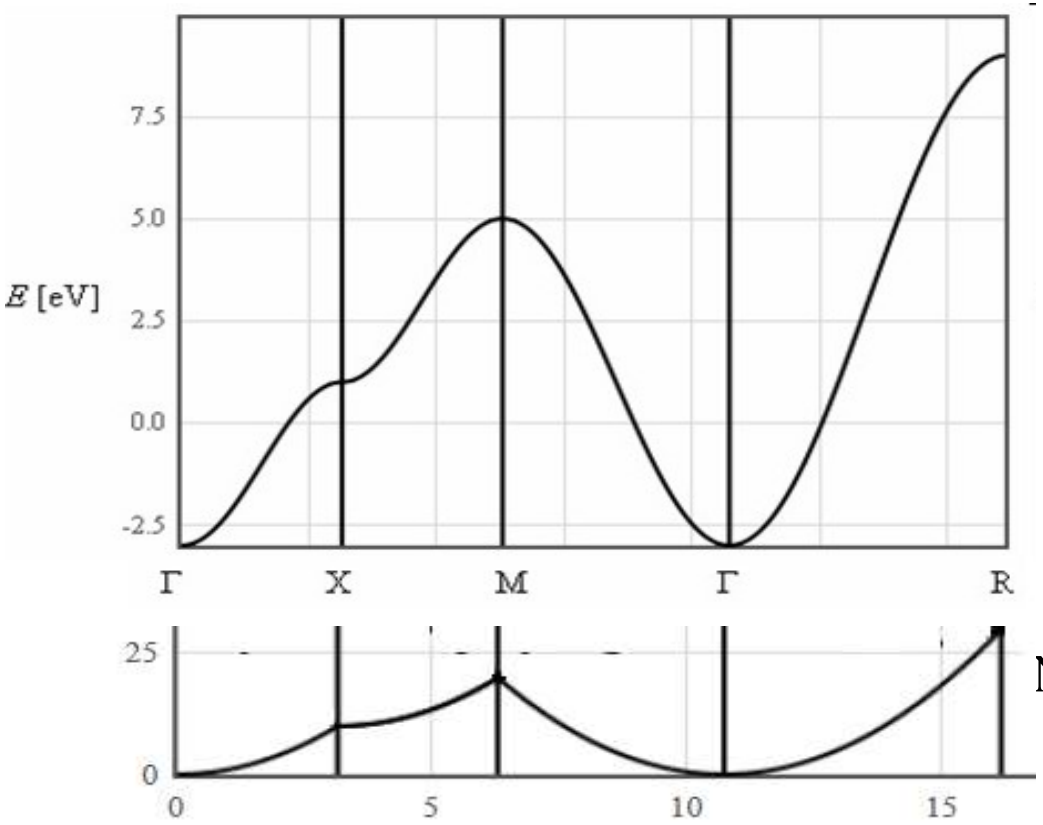
Overlap integral

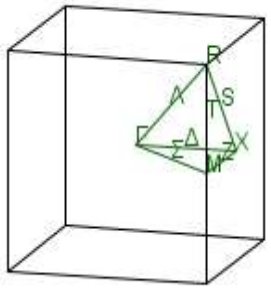
Tight binding, simple cubic

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

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

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

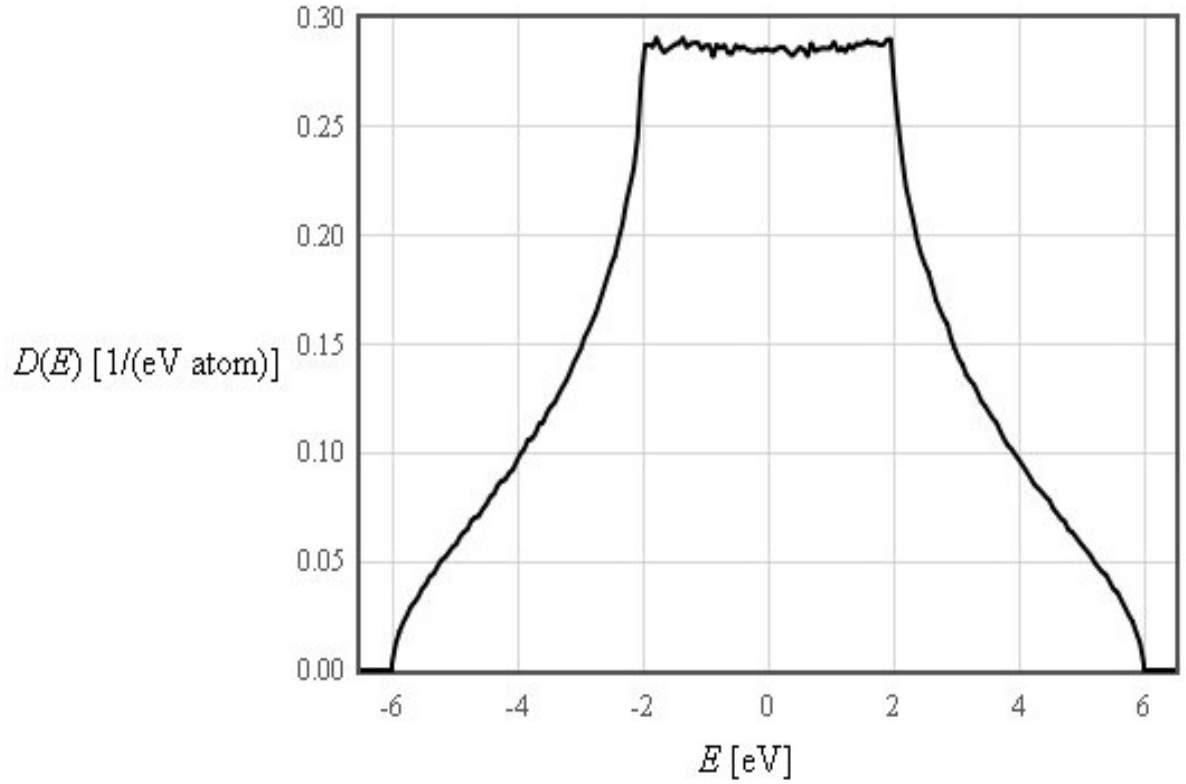




Effective mass $m^* = \dfrac{\hbar^2}{\dfrac{d^2E}{dk^2}} = \dfrac{\hbar^2}{2ta^2}$

Narrow bands → high effective mass

Density of states (simple cubic)



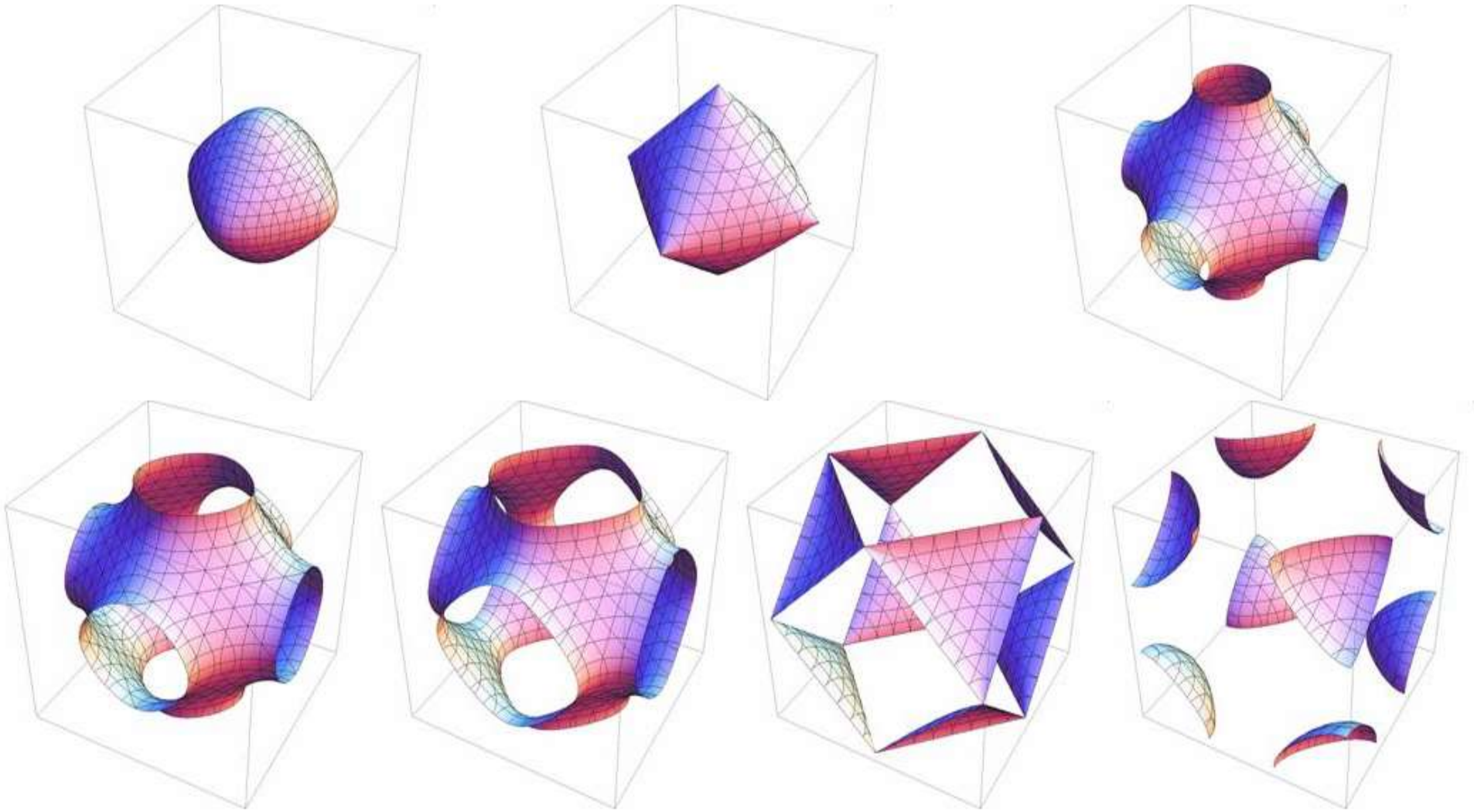
Calculate the energy for every allowed k in the Brillouin zone

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

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

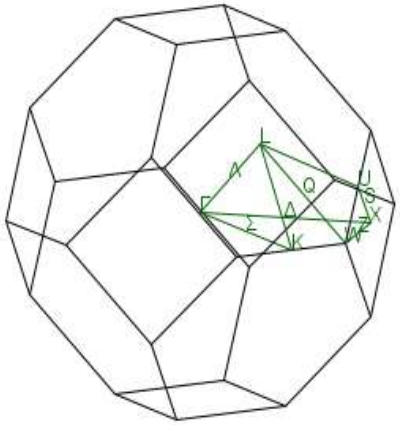
Tight binding, simple cubic

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



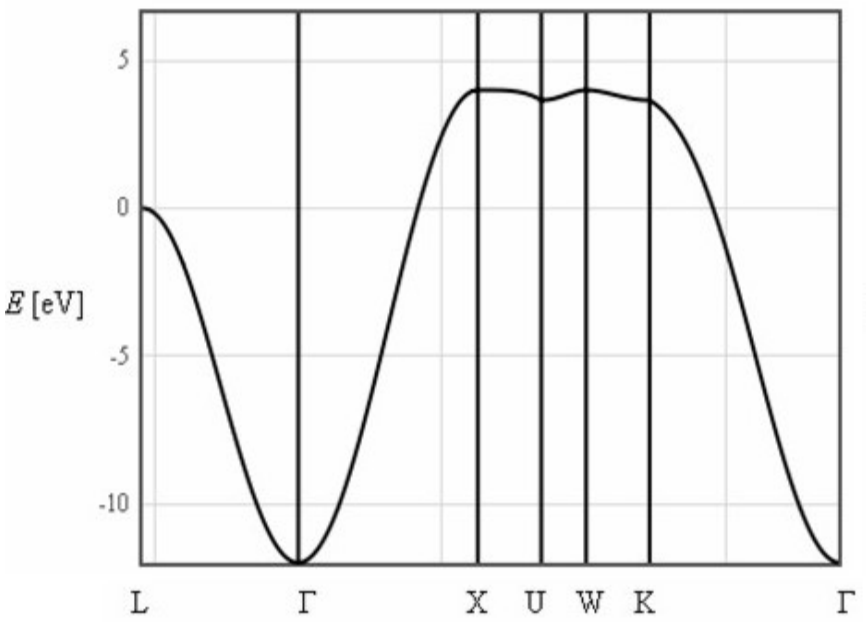
Christian Gruber, 2008

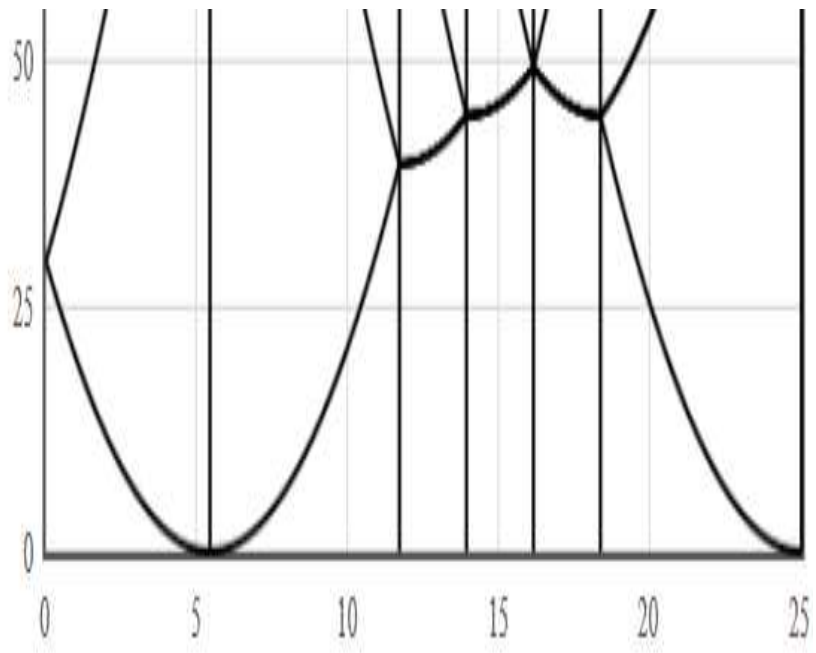
Tight binding, fcc



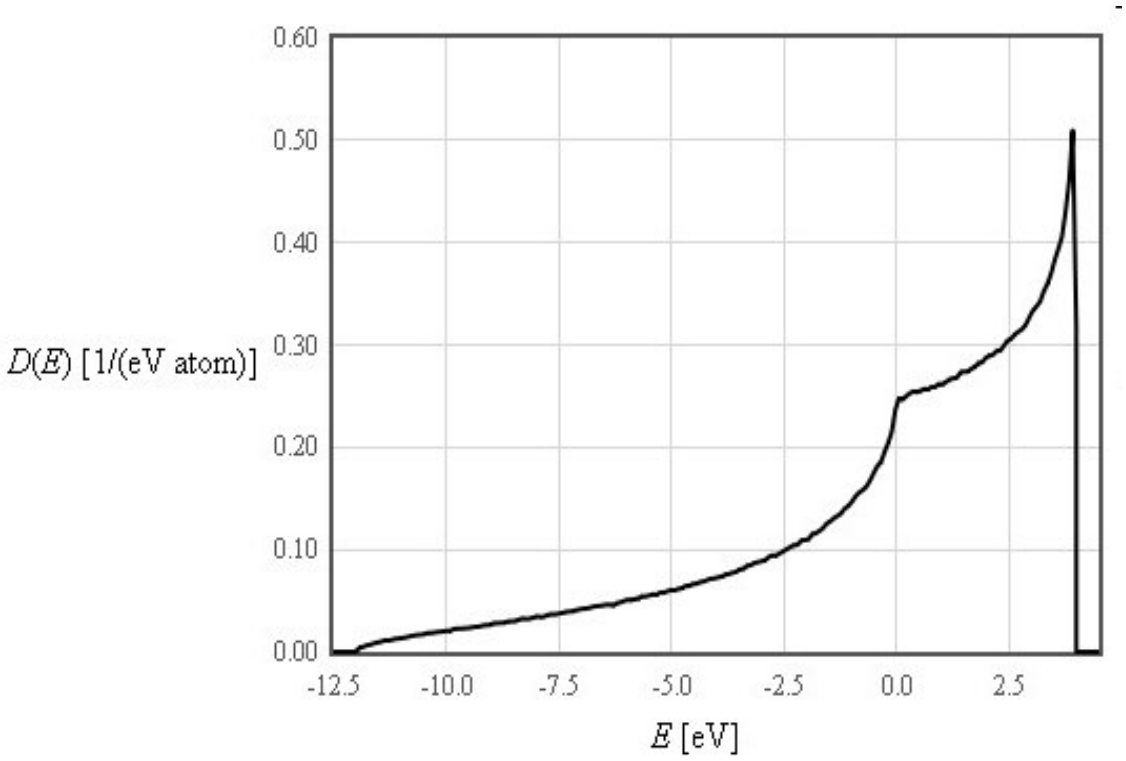
$$E = \varepsilon - t\sum_{lmn} e^{i\vec{k}\cdot\vec{\rho}_{lmn}}$$

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





Density of states (fcc)

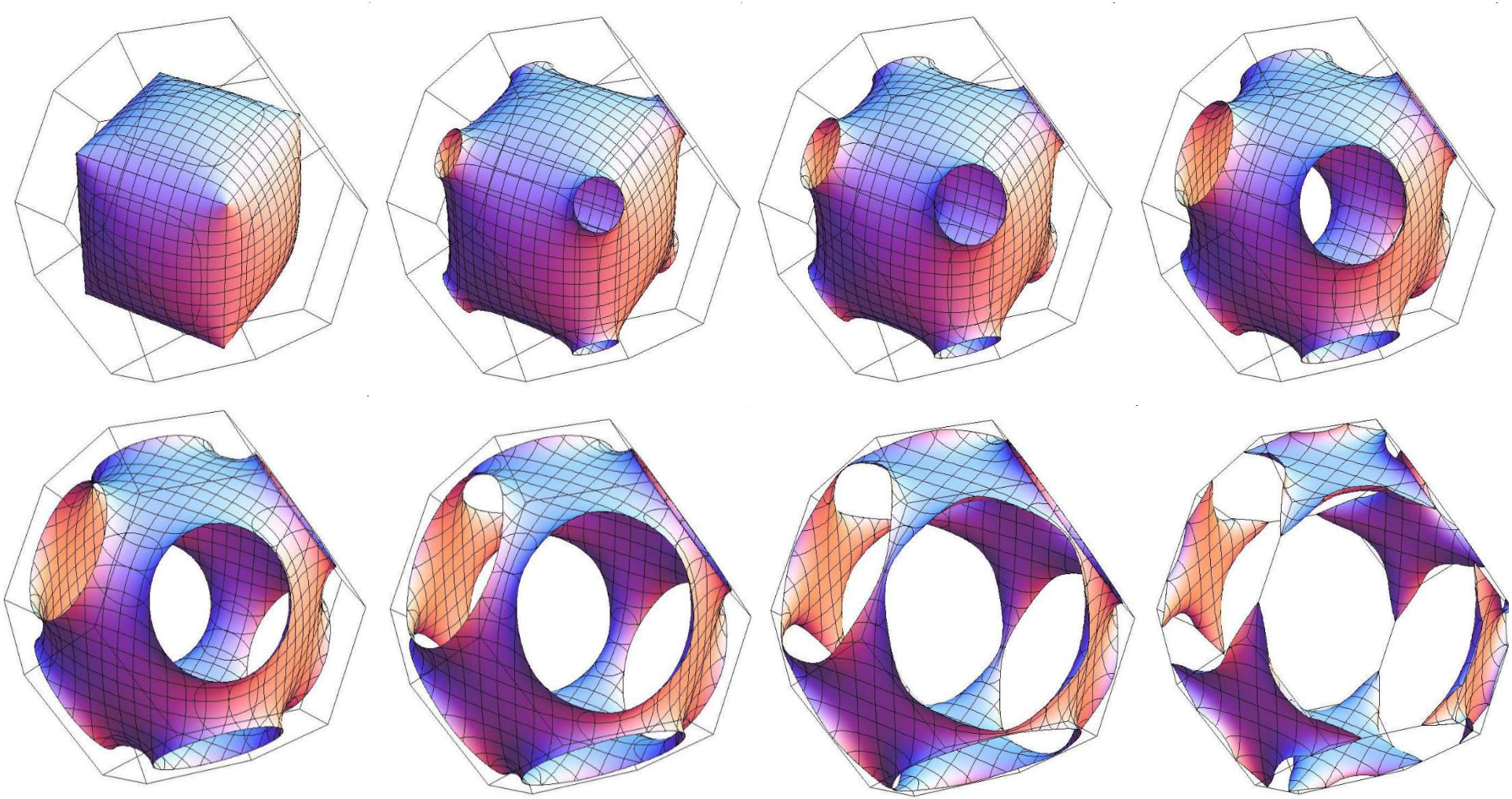


Calculate the energy for every allowed k in the Brillouin zone

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

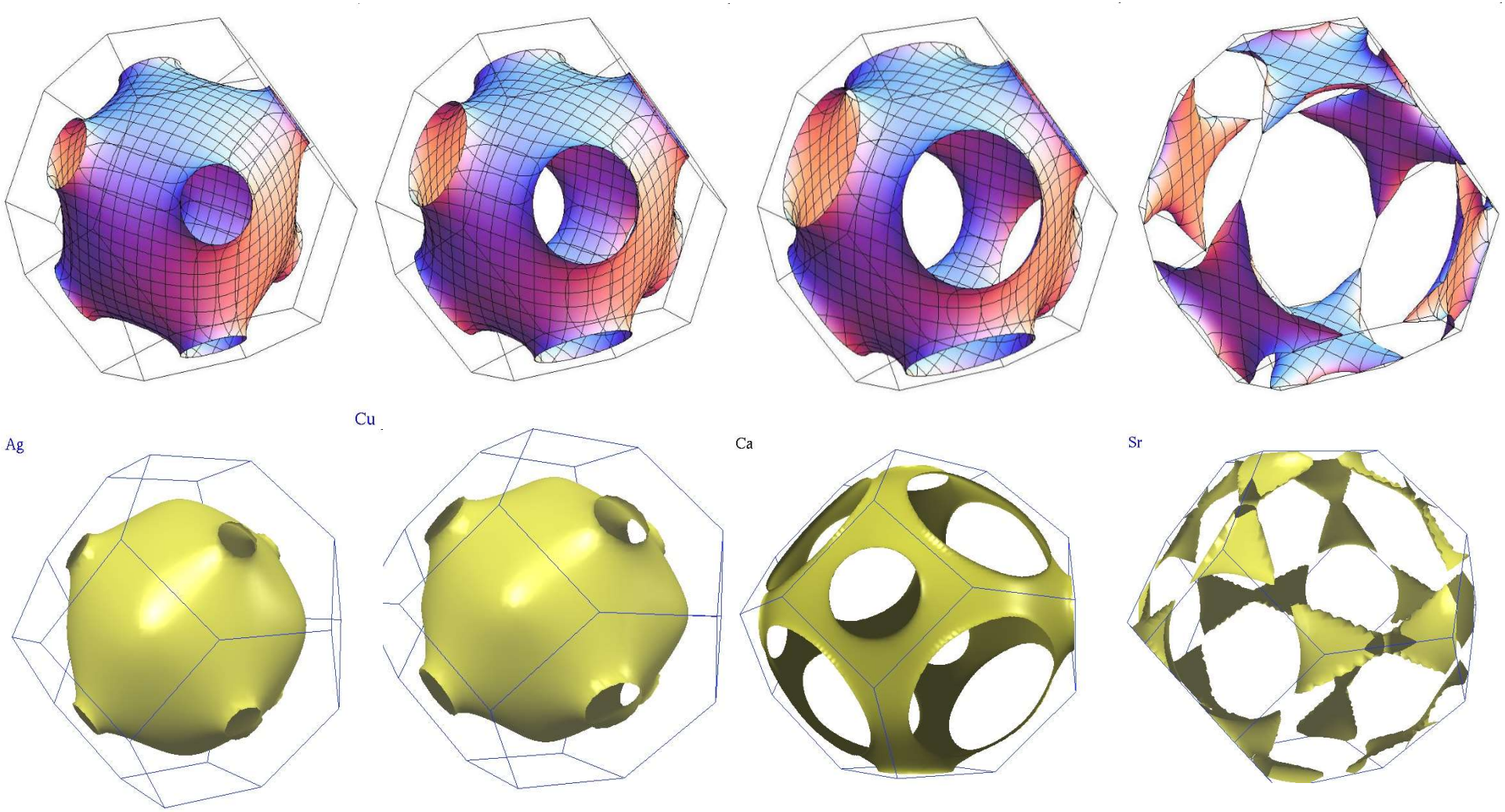
http://lamp.tu-graz.ac.at/~hadley/ss1/bands/tbtable/tbtable.html

Tight binding, fcc



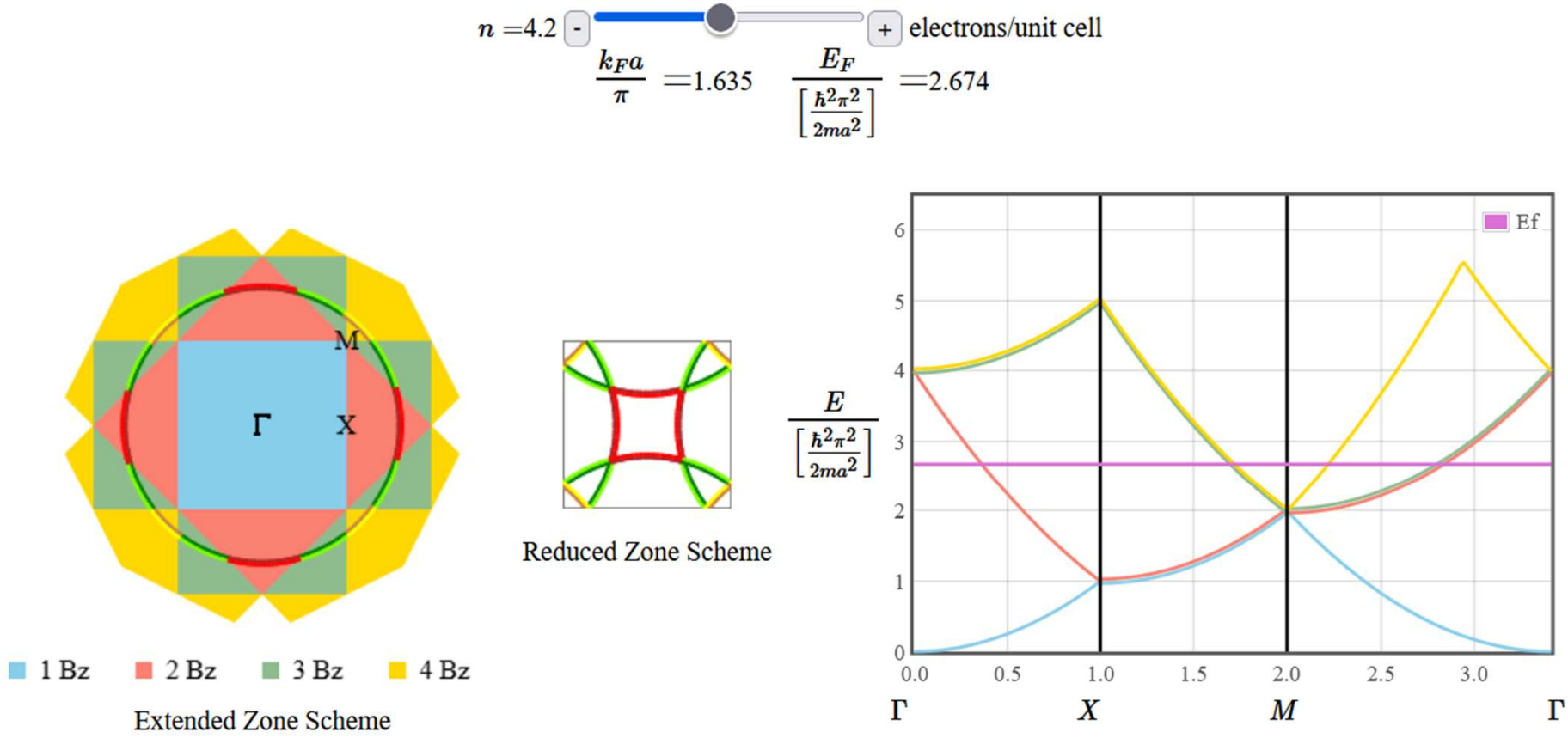
Christian Gruber, 2008

Tight binding, fcc



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

Fermi surface of a two-dimensional square lattice



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

Fermi Surfaces

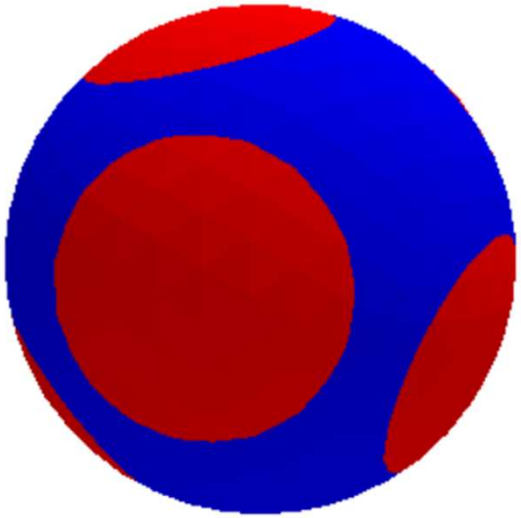
n =2 [-] [+] electrons/unit cell

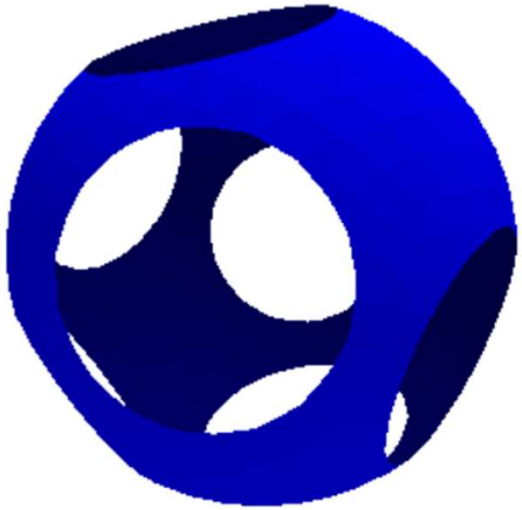
$k_F = (3\pi^2 n)^{1/3} = 3.90$

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

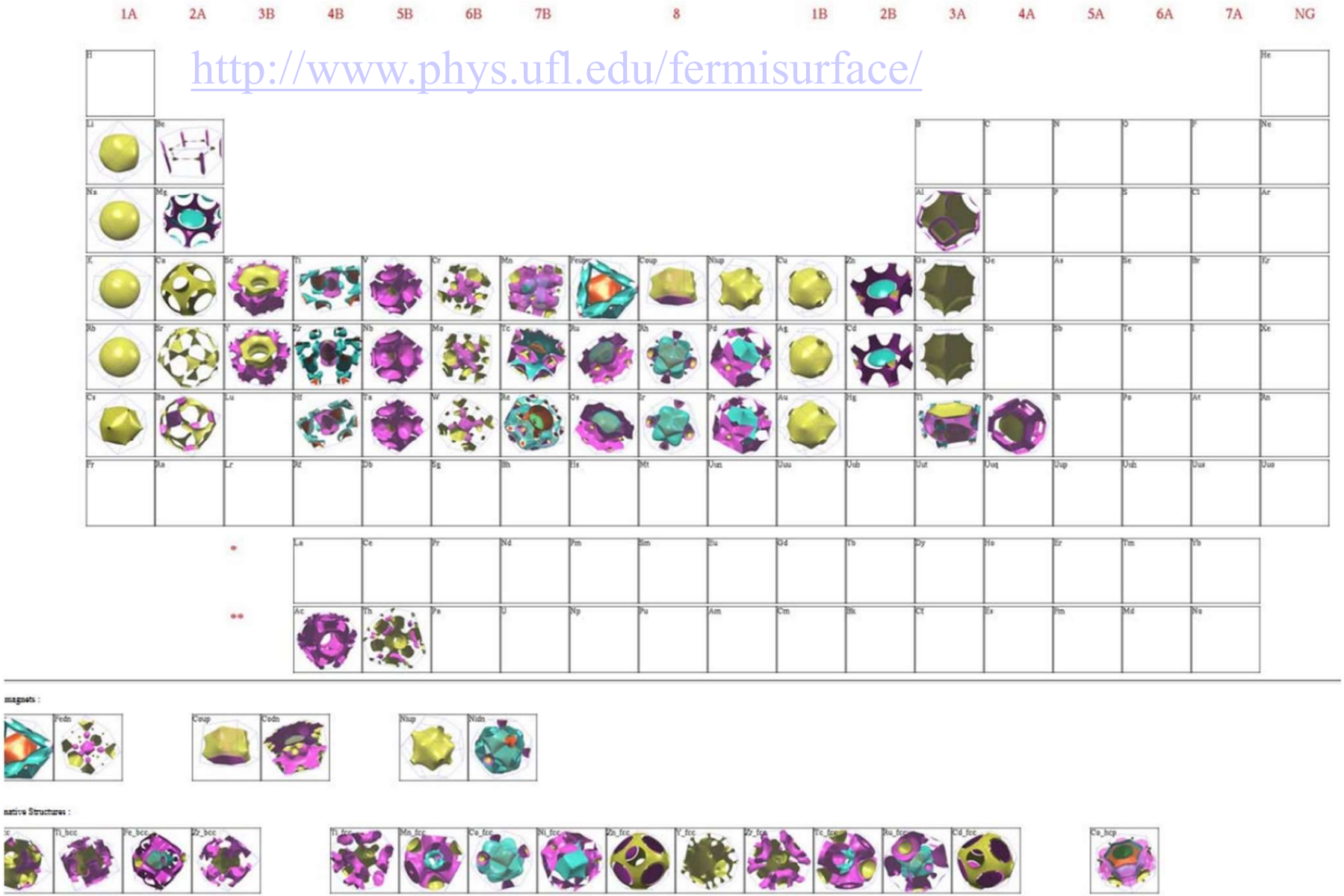
[Show 1st Brillouin zone] [Stop Rotation]

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





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


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 :