Band structure
Tight Binding
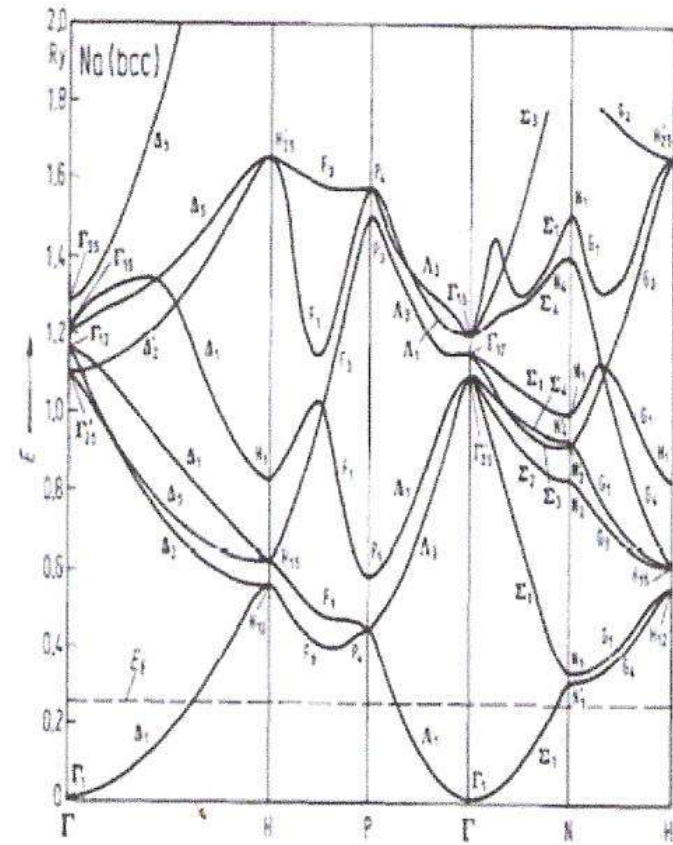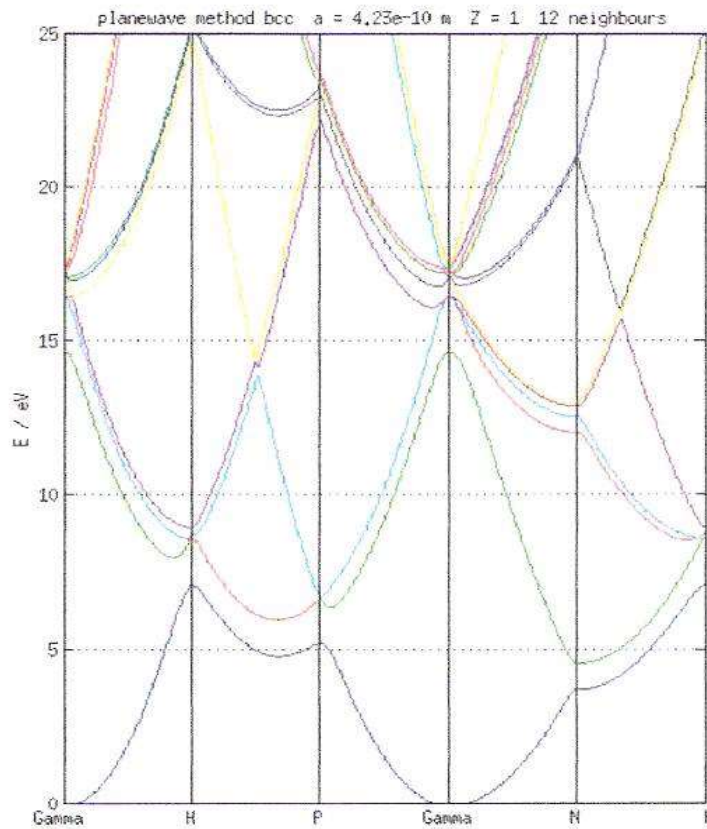
Plane wave method bcc

Abbildung 4: Planewave-Methode angewandt an Natrium vs. Literaturberechnung [1]

Muffin tin potentials, pseudopotentials

$$U(\vec{r}) = -\frac{Ze^2}{4\pi\varepsilon_0 r}$$ inside a radius R and is constant outside

$$U(\vec{r}) = \frac{Ze^2}{V\varepsilon_0} \sum_{\vec{G}} \left(\frac{\cos(|G|R) - 1}{|G|^2} + \frac{\sin(|G|R) - |G|R\cos(|G|R)}{|G|^3} \right) \exp(i\vec{G}\cdot\vec{r}).$$

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PSEUDOPOTENTIALS

Admin PP Database

More about pseudopotentials

Naming convention for the pseudopotential

Unified Pseudopotential Format

PSEUDOPOTENTIALS

Ready-to-use pseudopotentials are available from the periodic table below. Choose the options you desire from the menus (pseudopotentials from PSlibrary are recommended), then press "Filter". Elements for which at least a pseudopotential is available will appear in red. Click on the element entry and follow the link to access the pseudopotentials and a minimal description of their characteristics.

More information about pseudopotentials in general, the naming convention adopted for pseudopotential files, the Unified Pseudopotential Format , and on other pseudopotential databases, can be found via the links of the menu at the left.

Important Note: although most of these pseudopotentials were published or used with satisfactory results in published work, we cannot give any warranty whatsoever that they fit your actual needs.

ANY FUNCTIONAL ▾   ANY TYPE ▾   Apply Filter

ANY PP LIBRARY ▾   OTHER OPTIONS ▾

1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57-70	71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn

Si

Bachelor thesis Benedikt Tschofenig

a)

QUANTUMESPRESSO

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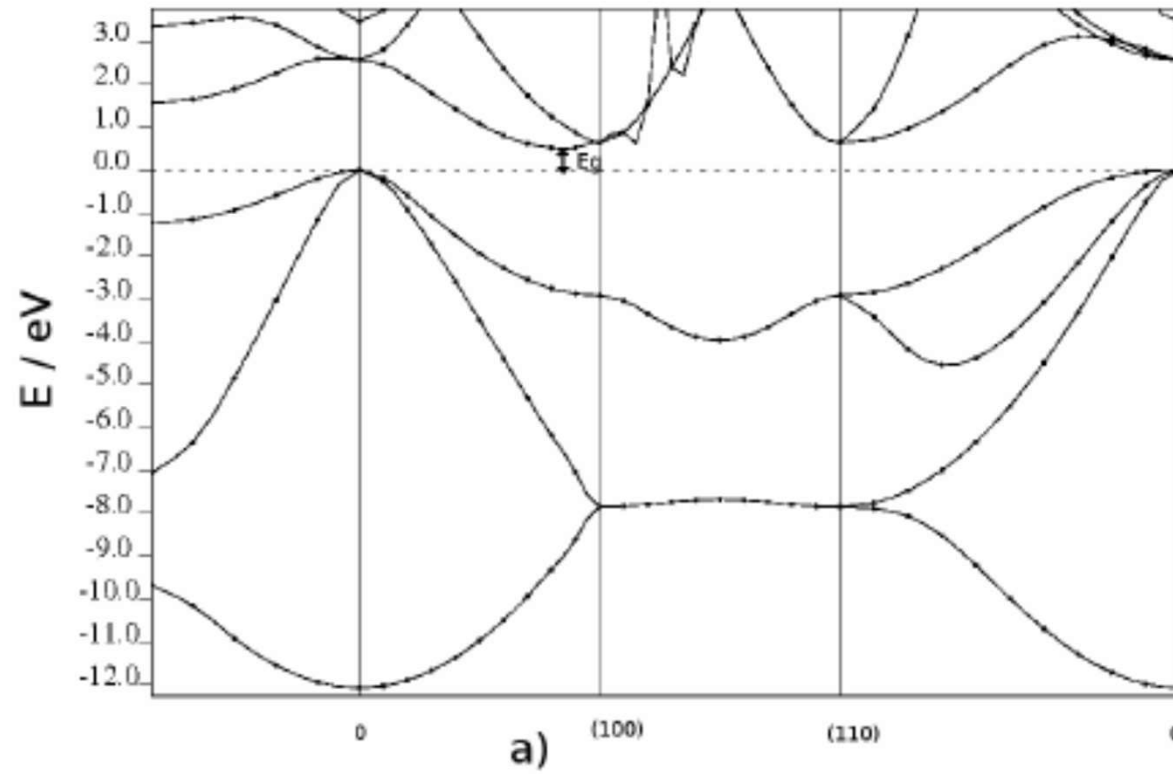
Tight binding

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

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

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

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

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

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

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

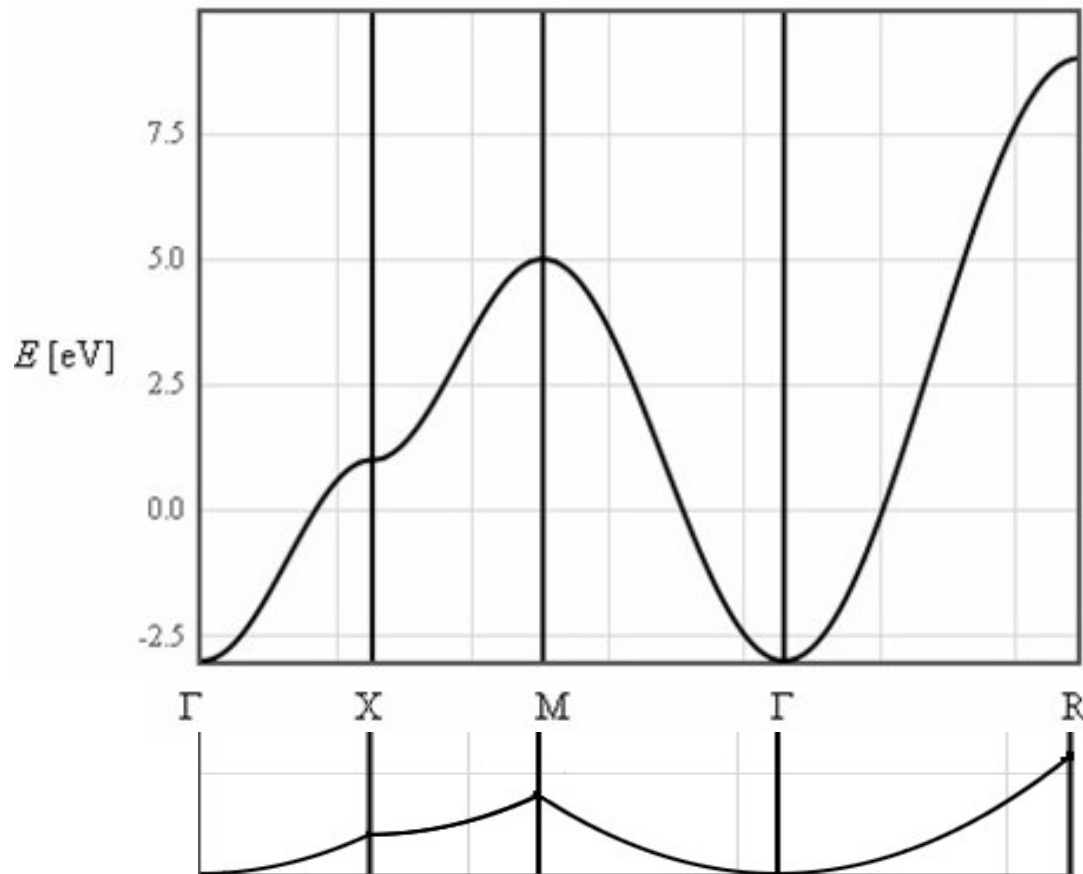$$\varepsilon = \langle \phi_a(\vec{r}) | H_{MO} | \phi_a(\vec{r}) \rangle \qquad\qquad t = -\langle \phi_a(\vec{r}) | H_{MO} | \phi_a(\vec{r} - \vec{\rho}_m) \rangle$$

Tight binding, simple cubic

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

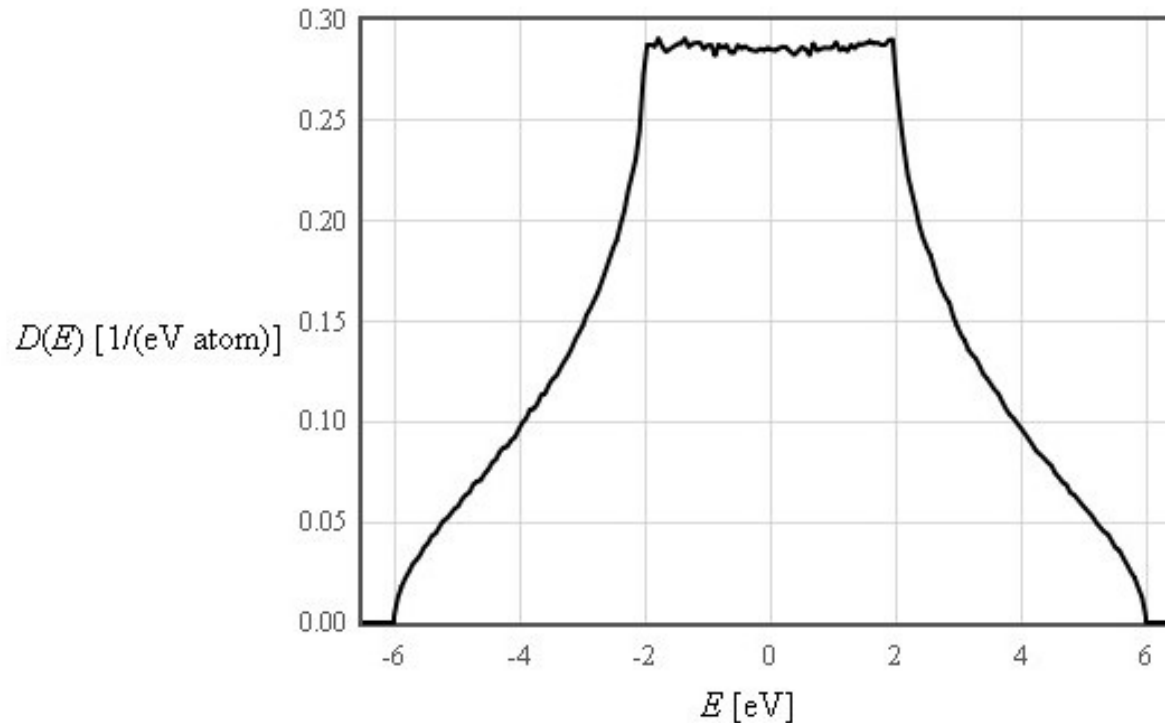$$E = \varepsilon - t\left(e^{ik_x a} + e^{-ik_x a} + e^{ik_y a} + e^{-ik_y a} + e^{ik_z a} + e^{-ik_z a}\right)$$

$$= \varepsilon - 2t\left(\cos(k_x a) + \cos(k_y a) + \cos(k_z a)\right)$$
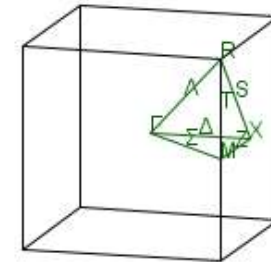
Effective mass $\quad m^* = \dfrac{\hbar^2}{\dfrac{d^2 E}{dk^2}} = \dfrac{\hbar^2}{2ta^2}$
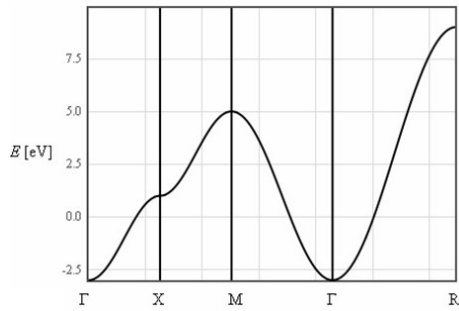
Narrow bands $\rightarrow$ high effective mass

Density of states (simple cubic)

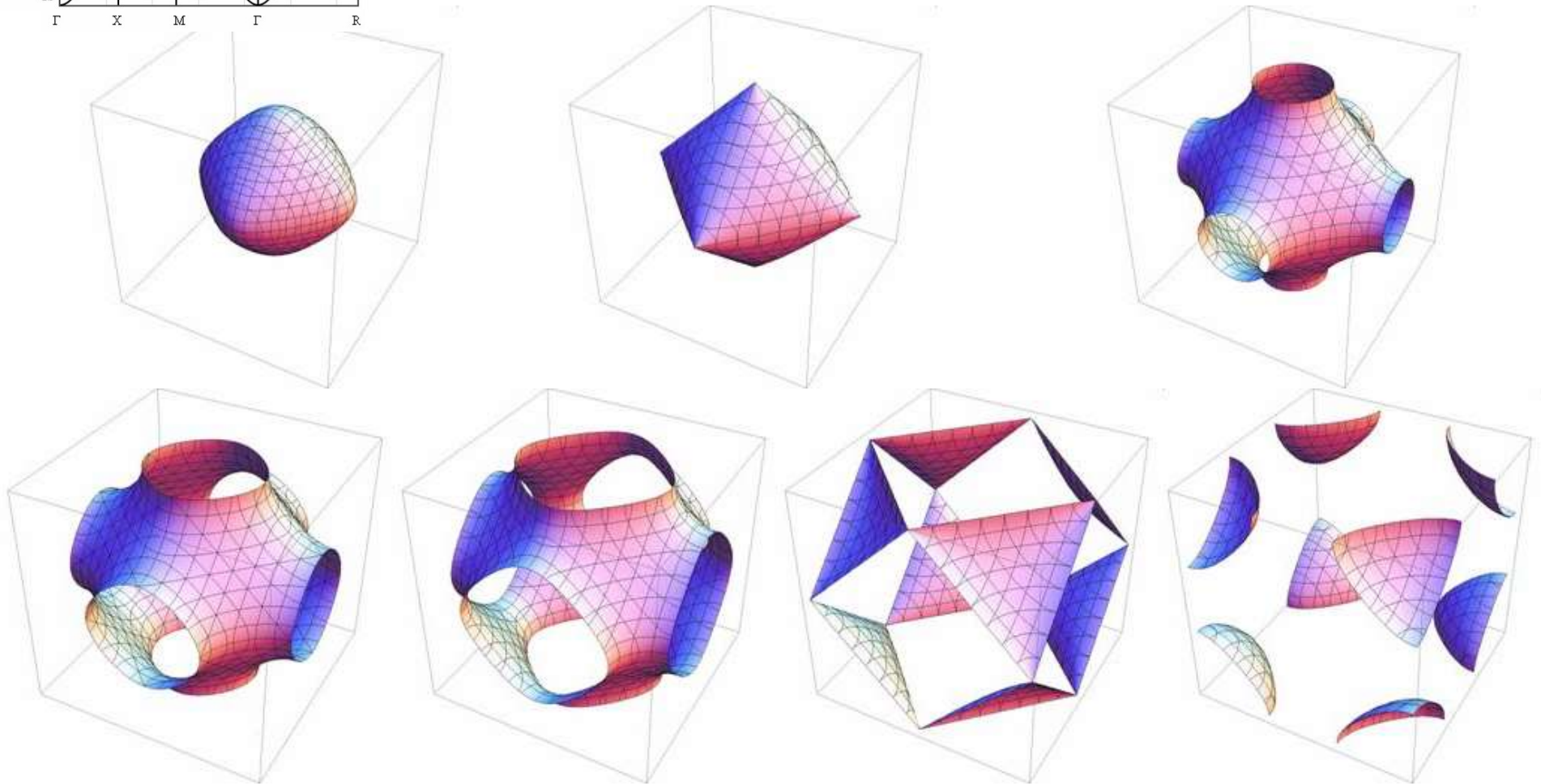Calculate the energy for every allowed k in the Brillouin zone

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

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

Tight binding, simple cubic

$$E = \varepsilon - 2t\left(\cos(k_x a) + \cos(k_y a) + \cos(k_z a)\right)$$
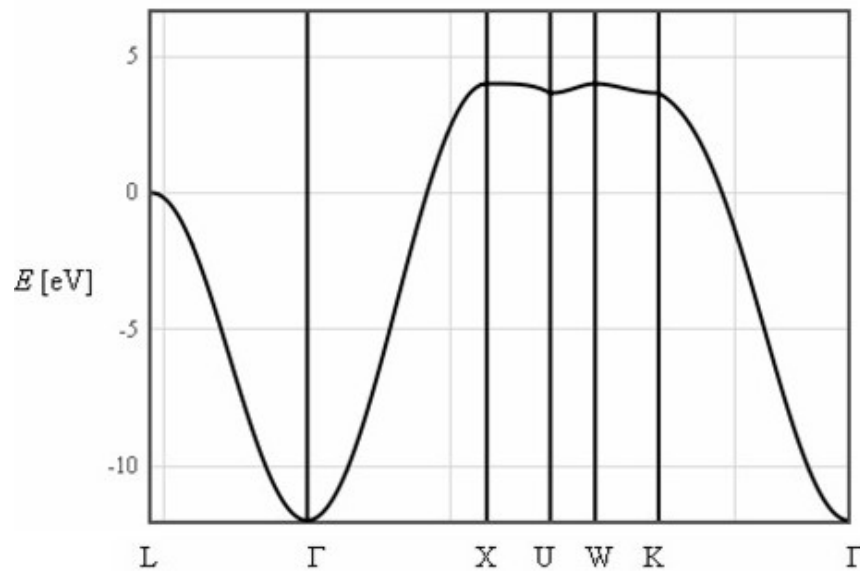
Christian Gruber, 2008

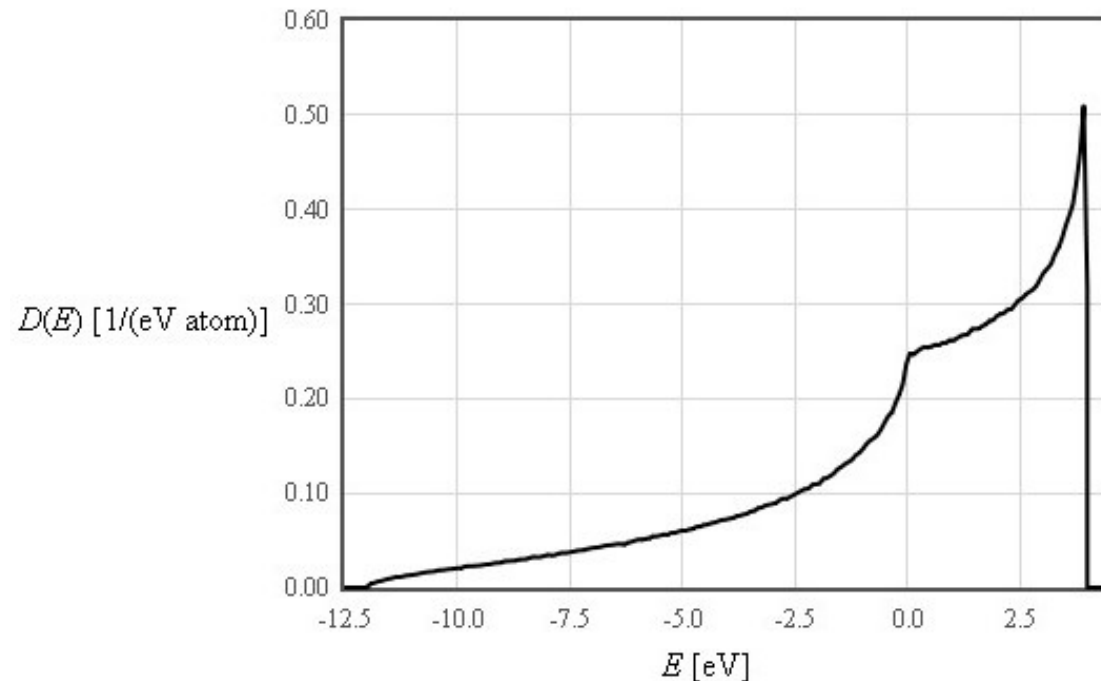# Tight binding, fcc

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

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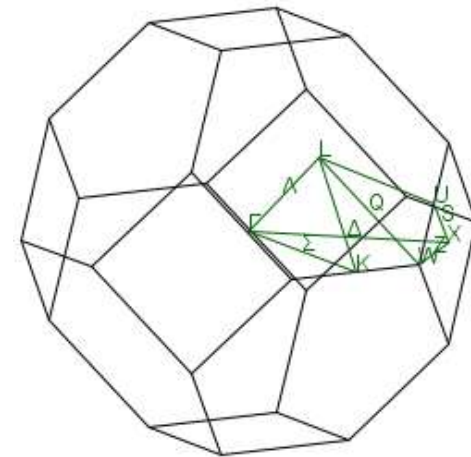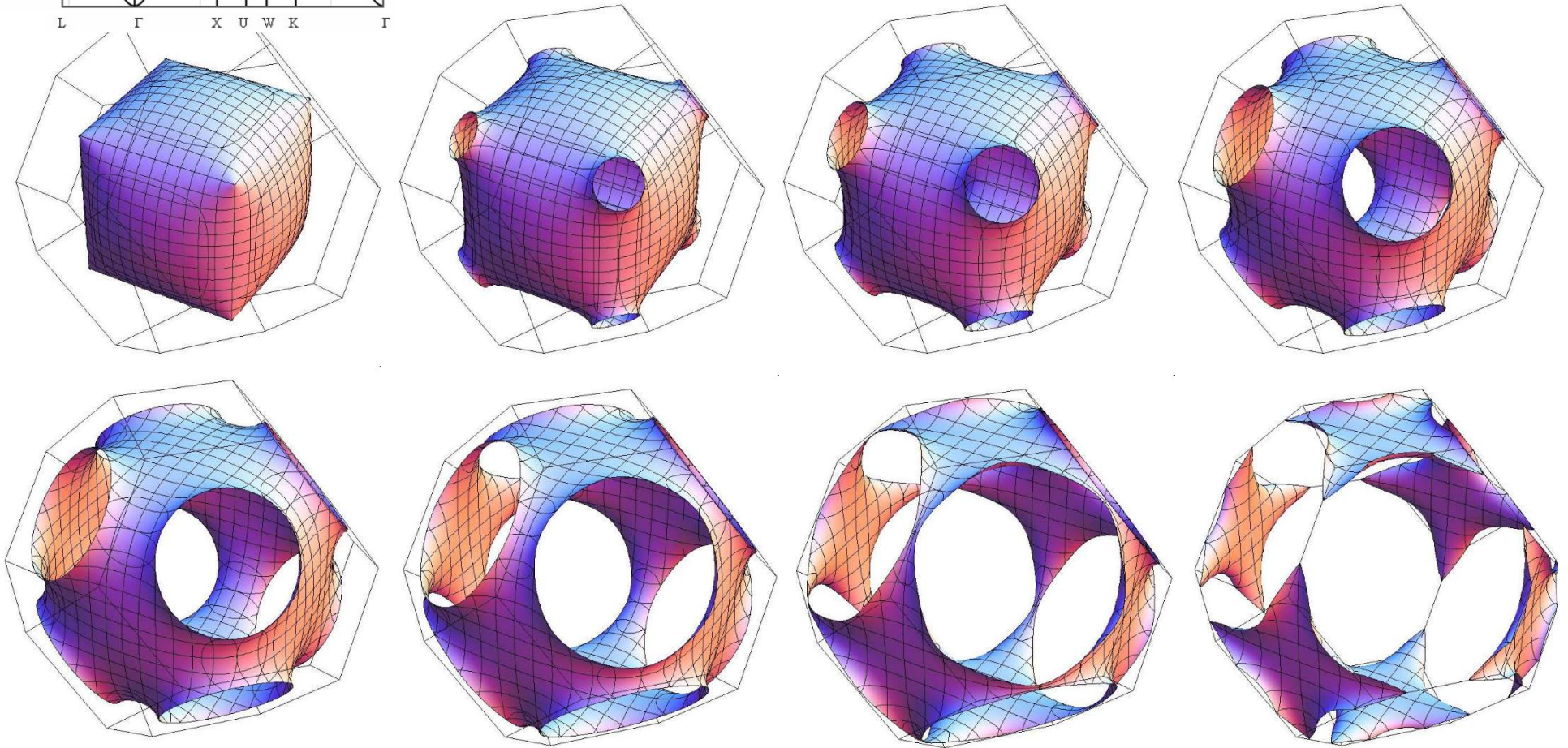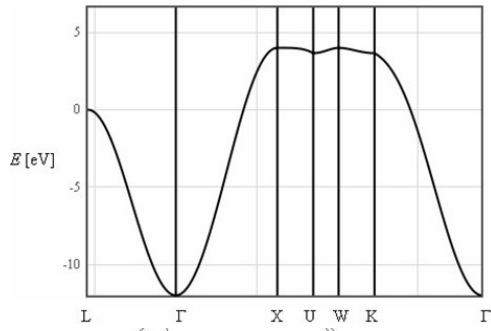
Density of states (fcc)

Calculate the energy for every allowed *k* in the Brillouin zone

$$E = \varepsilon - 4t\left(\cos\left(\frac{k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right) + \cos\left(\frac{k_x a}{2}\right)\cos\left(\frac{k_z a}{2}\right) + \cos\left(\frac{k_y a}{2}\right)\cos\left(\frac{k_z a}{2}\right)\right)$$
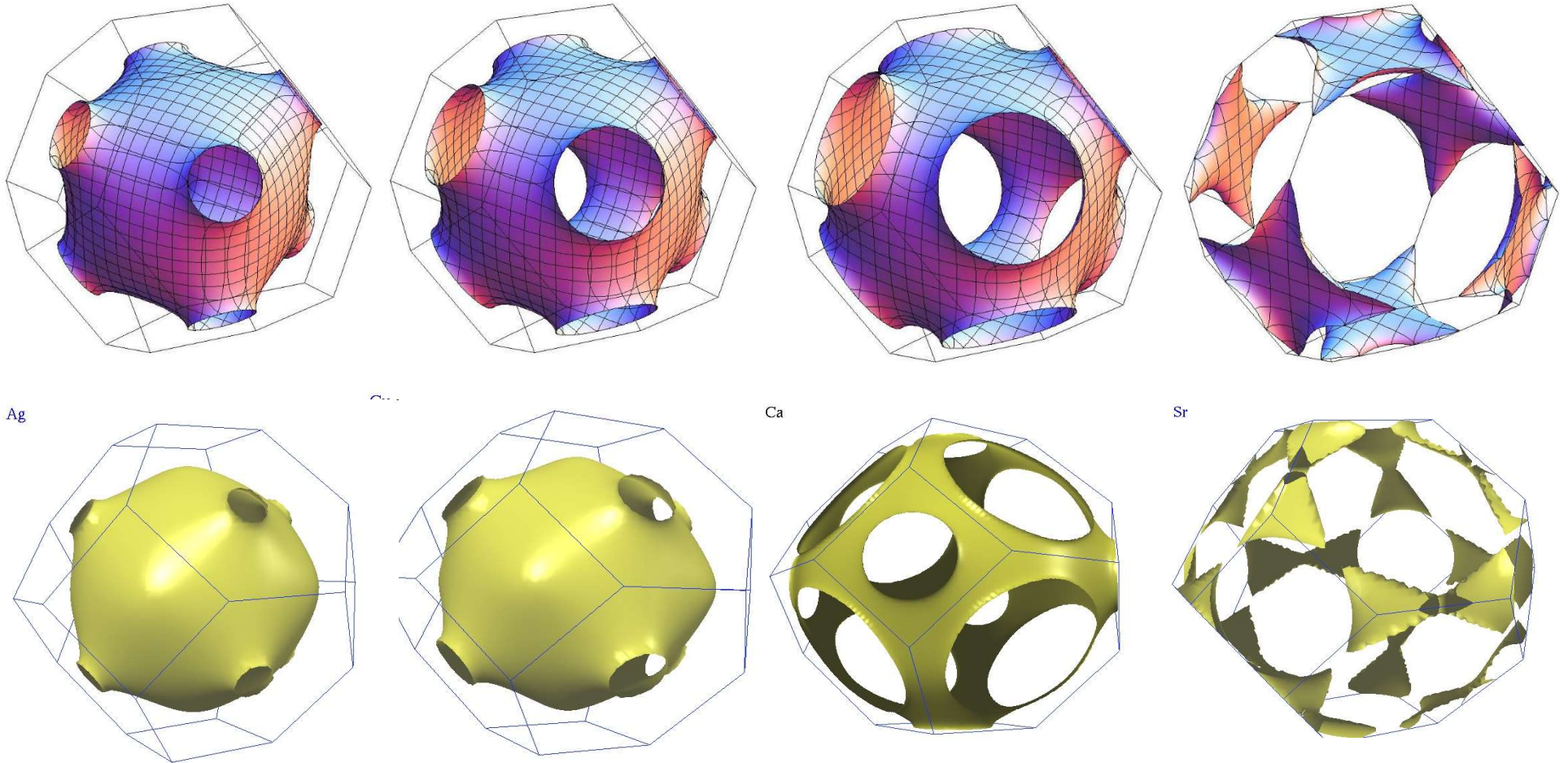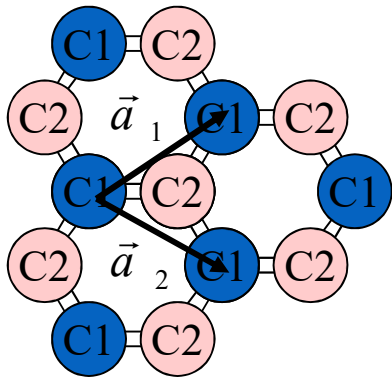
http://lamp.tu-graz.ac.at/~hadley/ss1/bands/tbtable/tbtable.html

Tight binding, fcc

Christian Gruber, 2008

Tight binding, fcc

Ag

Ca

Sr

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

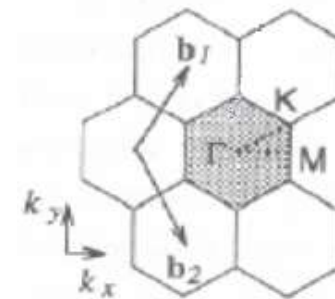# Graphene

$$\vec{a}_1 = \frac{\sqrt{3}}{2}a\hat{x} + \frac{1}{2}a\hat{y}$$

$$\vec{a}_2 = \frac{\sqrt{3}}{2}a\hat{x} - \frac{1}{2}a\hat{y}$$
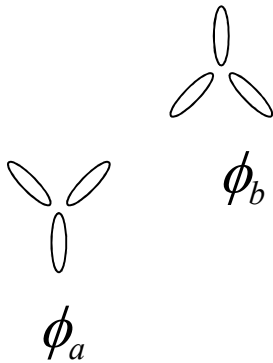

Two atoms per unit cell

Graphene has an unusual dispersion relation in the vicinity of the Fermi energy.

2 carbon atoms / unit cell

The standard guess for the wave function in the tight binding model is

$$\psi_k = \sum_{j,l} \exp\left(i\left(j\vec{k}\cdot\vec{a}_1 + l\vec{k}\cdot\vec{a}_2\right)\right)\left(c_a\phi_{p_za}\left(\vec{r} - j\vec{a}_1 - l\vec{a}_2\right) + c_b\phi_{p_zb}\left(\vec{r} - j\vec{a}_1 - l\vec{a}_2\right)\right)$$

For graphene, the valence orbitals are p_z orbitals

ϕ_b

Substitute this wave function into the Schrödinger equation

ϕ_a

$$H\psi_k = E\psi_k$$

2 carbon atoms / unit cell

$$\psi_k = \sum_{j,l} \exp\left(i\left(j\vec{k}\cdot\vec{a}_1 + l\vec{k}\cdot\vec{a}_2\right)\right)\left(c_a\phi_{p_za}\left(\vec{r}-j\vec{a}_1-l\vec{a}_2\right)+c_b\phi_{p_zb}\left(\vec{r}-j\vec{a}_1-l\vec{a}_2\right)\right)$$

$$H\psi_k = E\psi_k$$

Multiply by $\phi^*_{p_za}(\vec{r})$ and integrate

the orbital for the atom at $j = 0, l = 0$.

$$c_a\langle\phi_a|H|\phi_a\rangle + c_b\langle\phi_a|H|\phi_b\rangle\sum_m e^{i\vec{k}\cdot\vec{\rho}_m} + \text{small terms}$$

$$= E\left(c_a\langle\phi_a|\phi_a\rangle + c_b\langle\phi_a|\phi_b\rangle\sum_m e^{i\vec{k}\cdot\vec{\rho}_m} + \text{small terms}\right)$$

1   0

m sums over the nearest neighbors

2 carbon atoms / unit cell

To get a second equation for c_a and c_b

Multiply $H\psi_k = E\psi_k$ by $\phi^*_{p_z b}(\vec{r})$ and integrate

the orbital for the atom at $j = 0$, $l = 0$.

$$c_a \left\langle \phi_b \left| H \right| \phi_a \right\rangle \sum_m e^{-i\vec{k}\cdot\vec{\rho}_m} + c_b \left\langle \phi_b \left| H \right| \phi_b \right\rangle + \text{small terms}$$

$$= E\left(c_a \left\langle \phi_b \middle| \phi_a \right\rangle \sum_m e^{i\vec{k}\cdot\vec{\rho}_m} + c_b \left\langle \phi_b \middle| \phi_b \right\rangle + \text{small terms} \right)$$

$$0 \qquad\qquad\qquad 1$$

Write as a matrix equation

Tight binding graphene

$$
\begin{bmatrix}
\langle \phi_a | H | \phi_a \rangle - E & \langle \phi_a | H | \phi_b \rangle \sum_m e^{i \vec{k} \cdot \vec{\rho}_m} \\
\langle \phi_b | H | \phi_a \rangle \sum_m e^{-i \vec{k} \cdot \vec{\rho}_m} & \langle \phi_b | H | \phi_b \rangle - E
\end{bmatrix}
\begin{bmatrix}
c_a \\
c_b
\end{bmatrix} = 0
$$

m sums over the nearest neighbors.

There will be two eigen energies for every *k*.

N orbitals / unit cell results in *N* bands

$$
\varepsilon = \langle \phi_a | H | \phi_a \rangle
$$

$$
t = - \langle \phi_a | H | \phi_b \rangle
$$