Tight binding

Tight binding does not include electron-electron interactions

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

Assume a solution of the form.

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

atomic orbitals: choose the relevant valence orbitals

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

Tight binding

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

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

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

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

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

There is one equation for each atomic orbital

Tight binding, one atomic orbital

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

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

For only one atomic orbital in the sum over valence orbitals

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

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

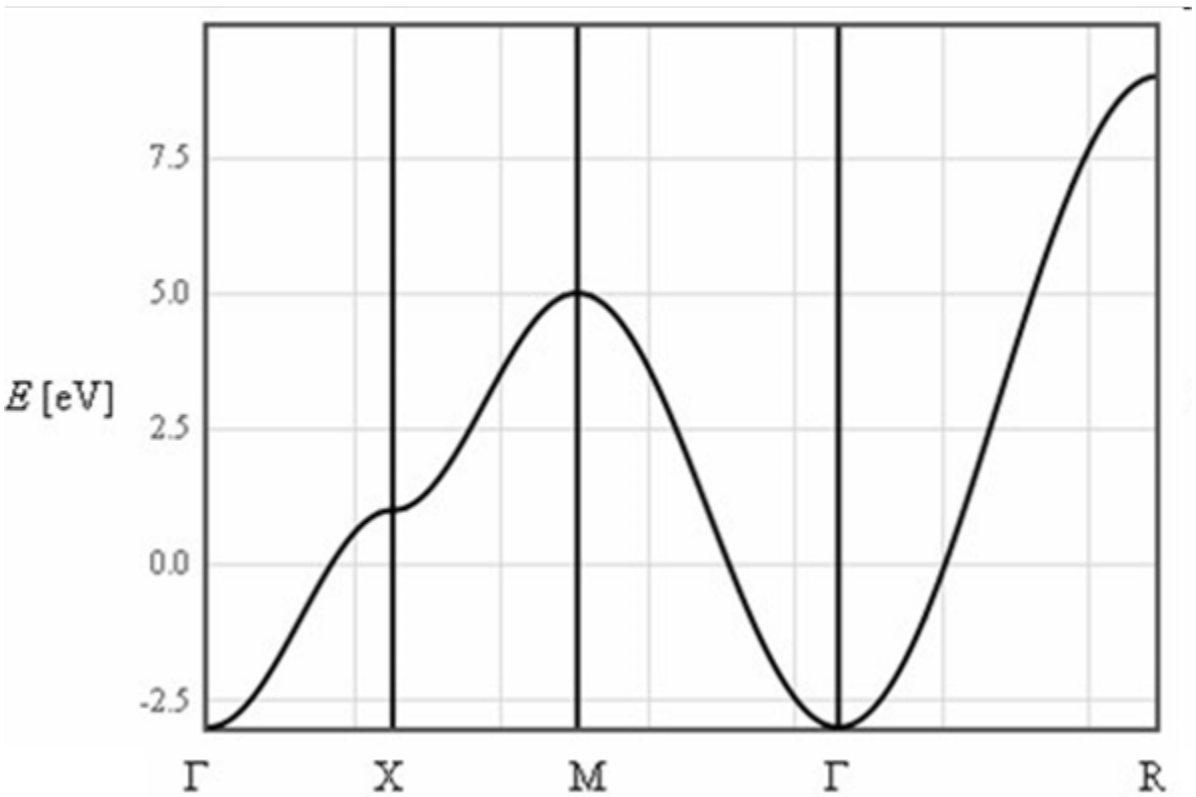
$$\varepsilon = \langle \psi_a(\vec{r}) | H_{MO} | \psi_a(\vec{r}) \rangle \qquad t = -\langle \psi_a(\vec{r}) | H_{MO} | \psi_a(\vec{r} - \vec{\rho}_m) \rangle$$

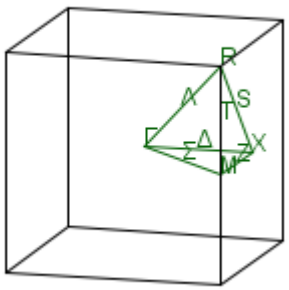
Tight binding, simple cubic

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

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

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

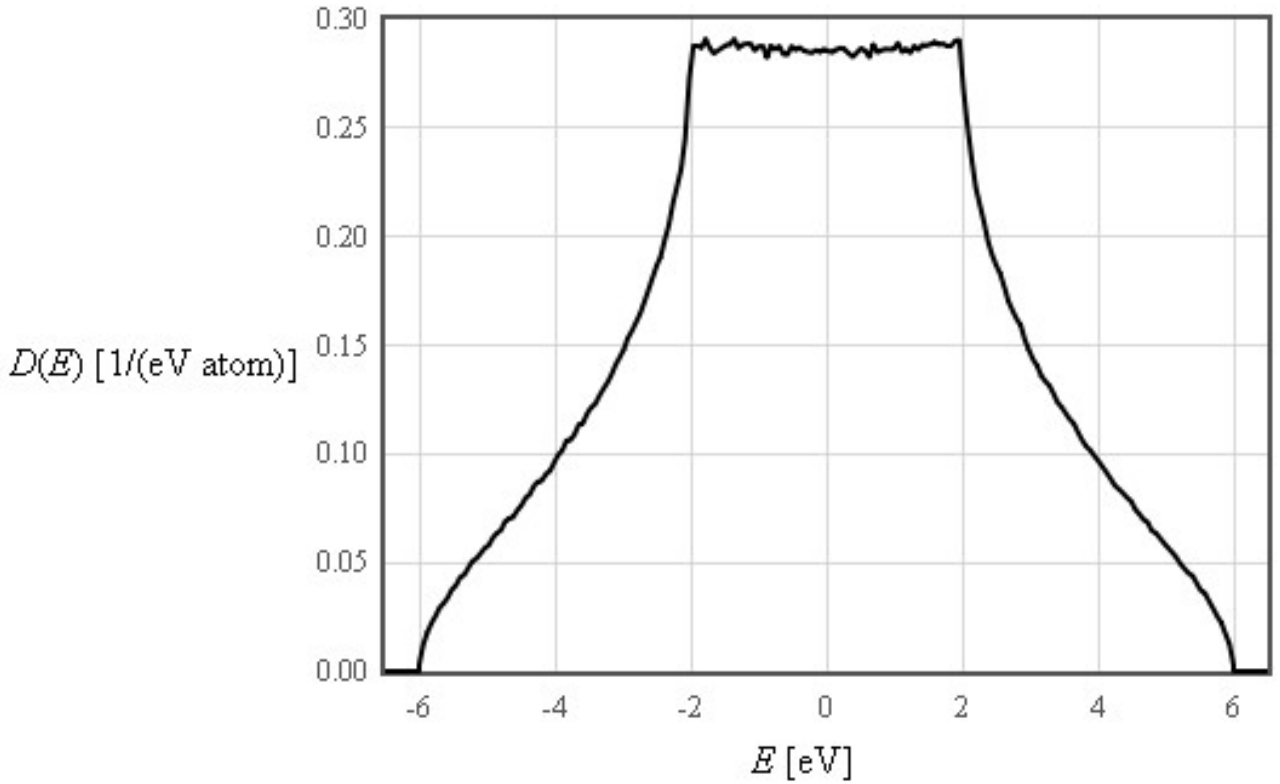




Effective mass $m^* = \dfrac{\hbar^2}{\dfrac{d^2E}{dk^2}} = \dfrac{\hbar^2}{2ta^2}$

Narrow bands → high effective mass

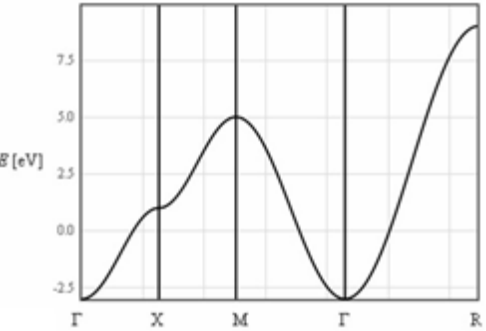
Density of states (simple cubic)



Calculate the energy for every allowed k in the Brillouin zone

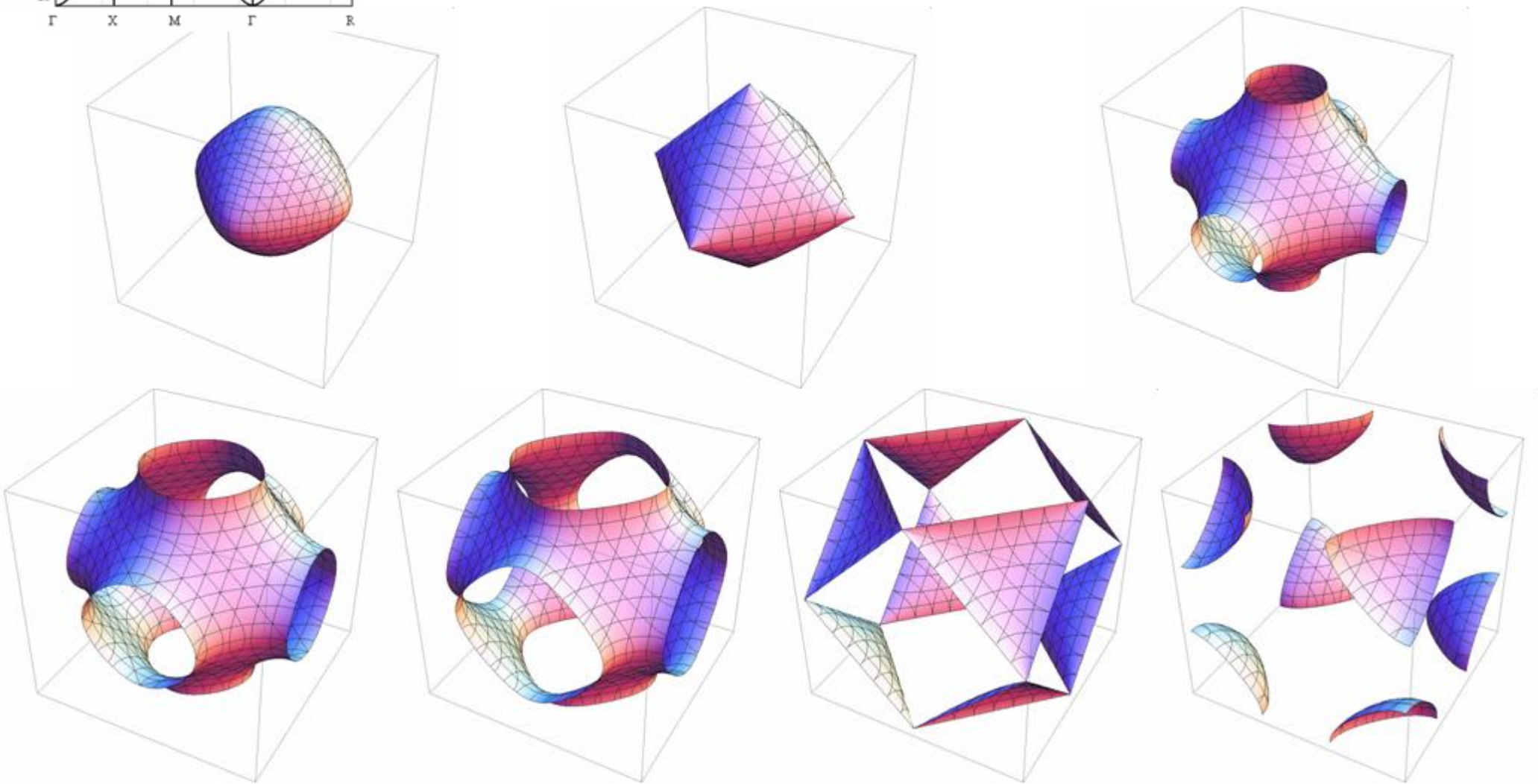
$$E = \varepsilon - 2t\left(\cos(k_x a) + \cos(k_y a) + \cos(k_z a)\right)$$

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



Tight binding, simple cubic

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

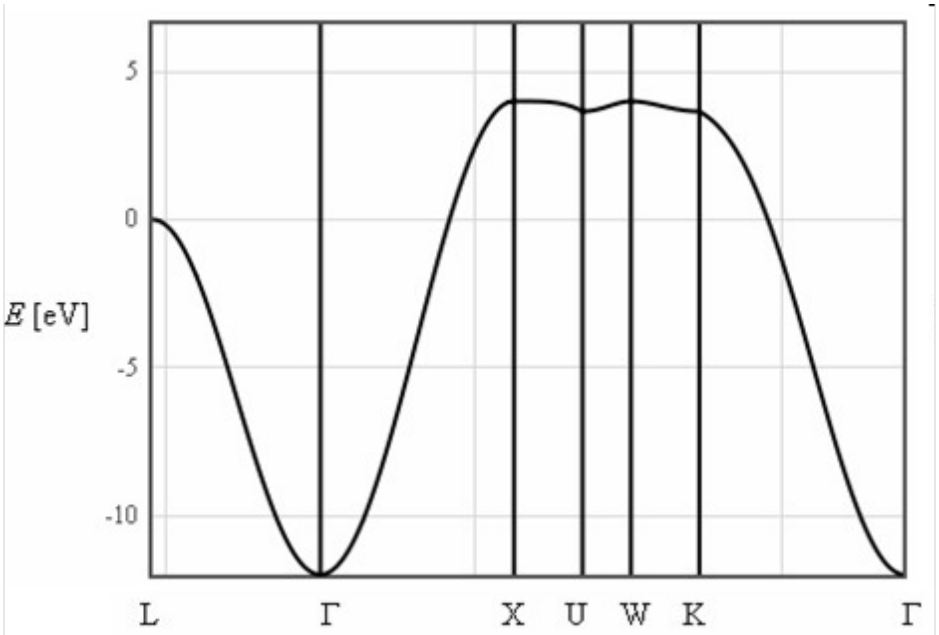


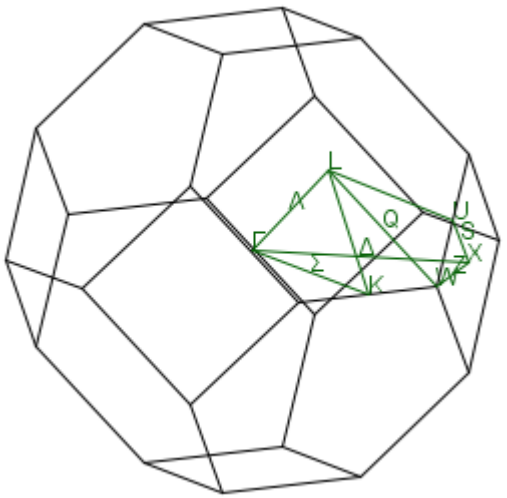
Christian Gruber, 2008

Tight binding, fcc

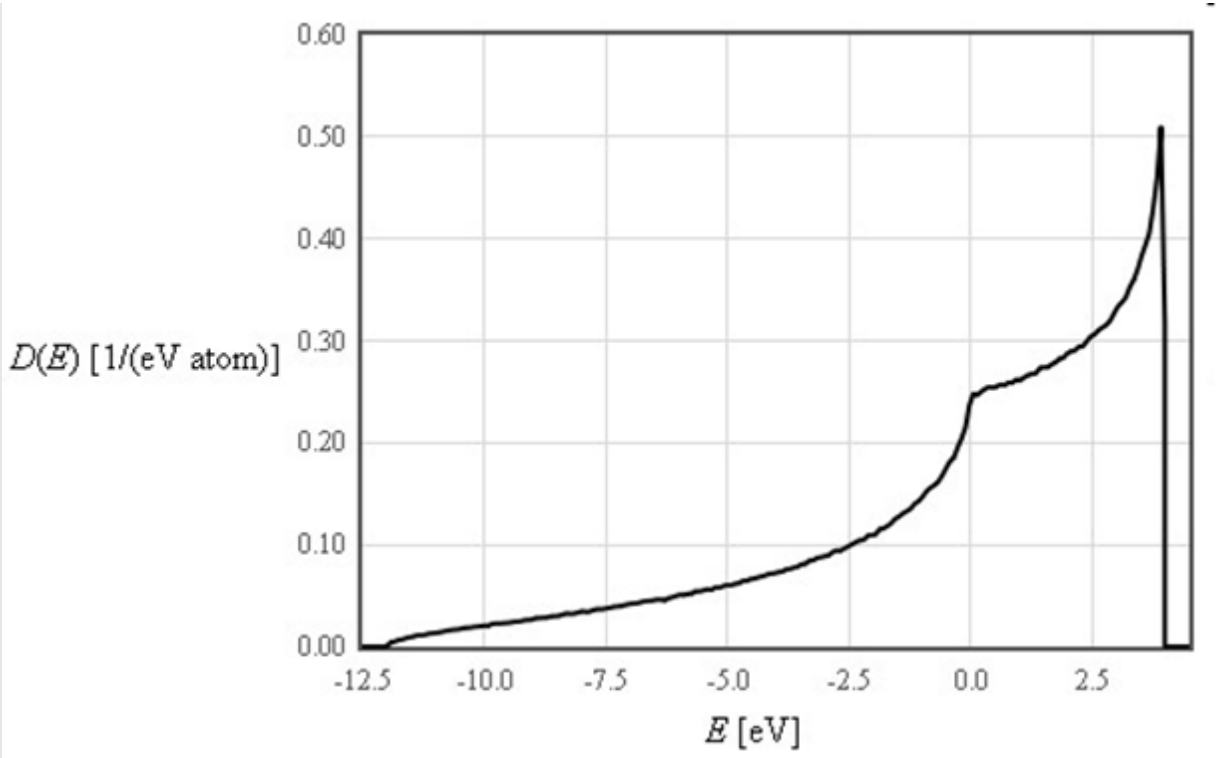
$$E = \varepsilon - t\sum_{m} e^{i\vec{k}\cdot\vec{\rho}_m}$$

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





Density of states (fcc)

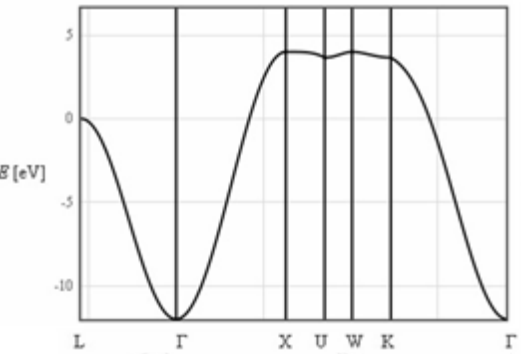


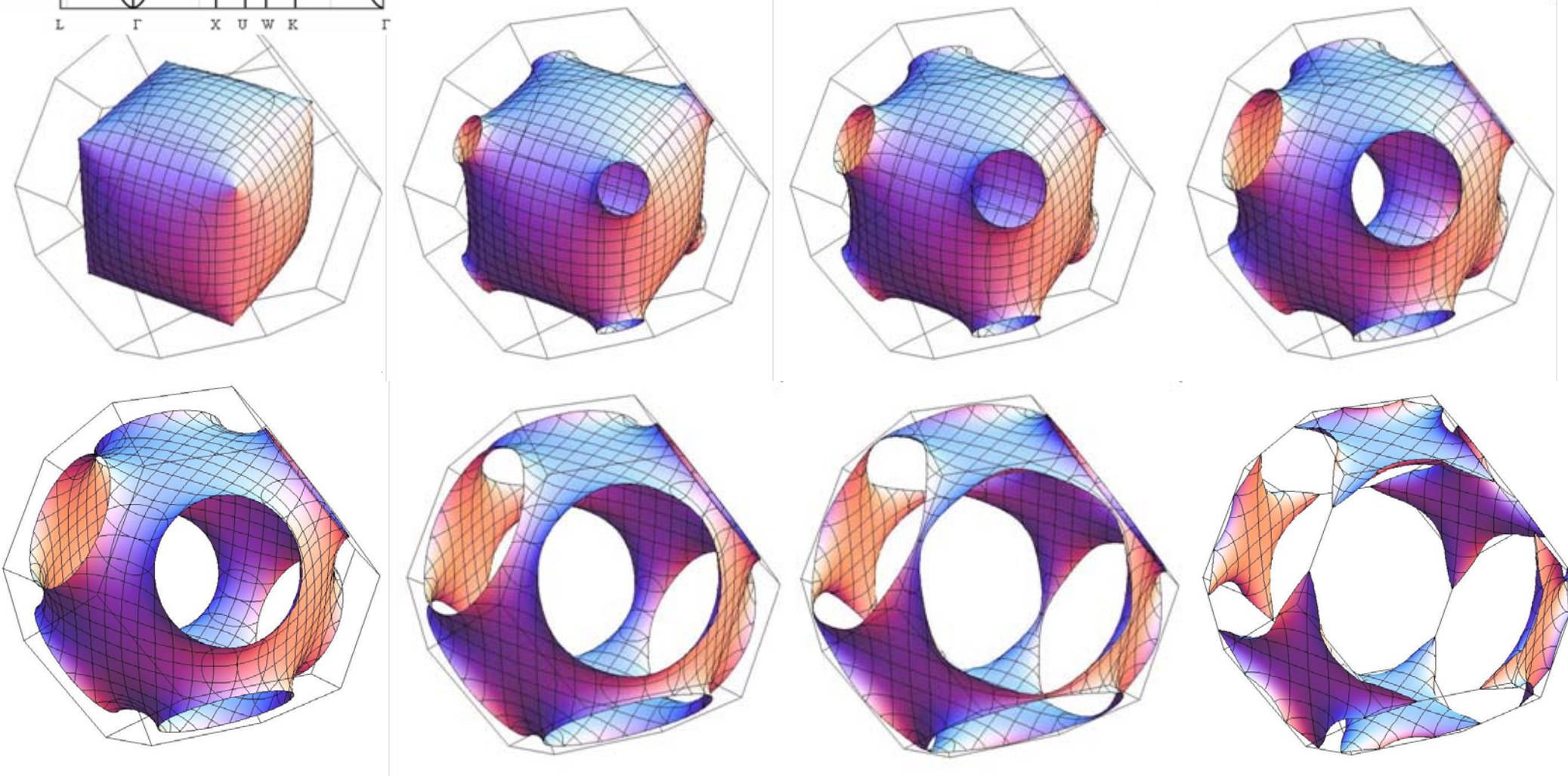
Calculate the energy for every allowed *k* in the Brillouin zone

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

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

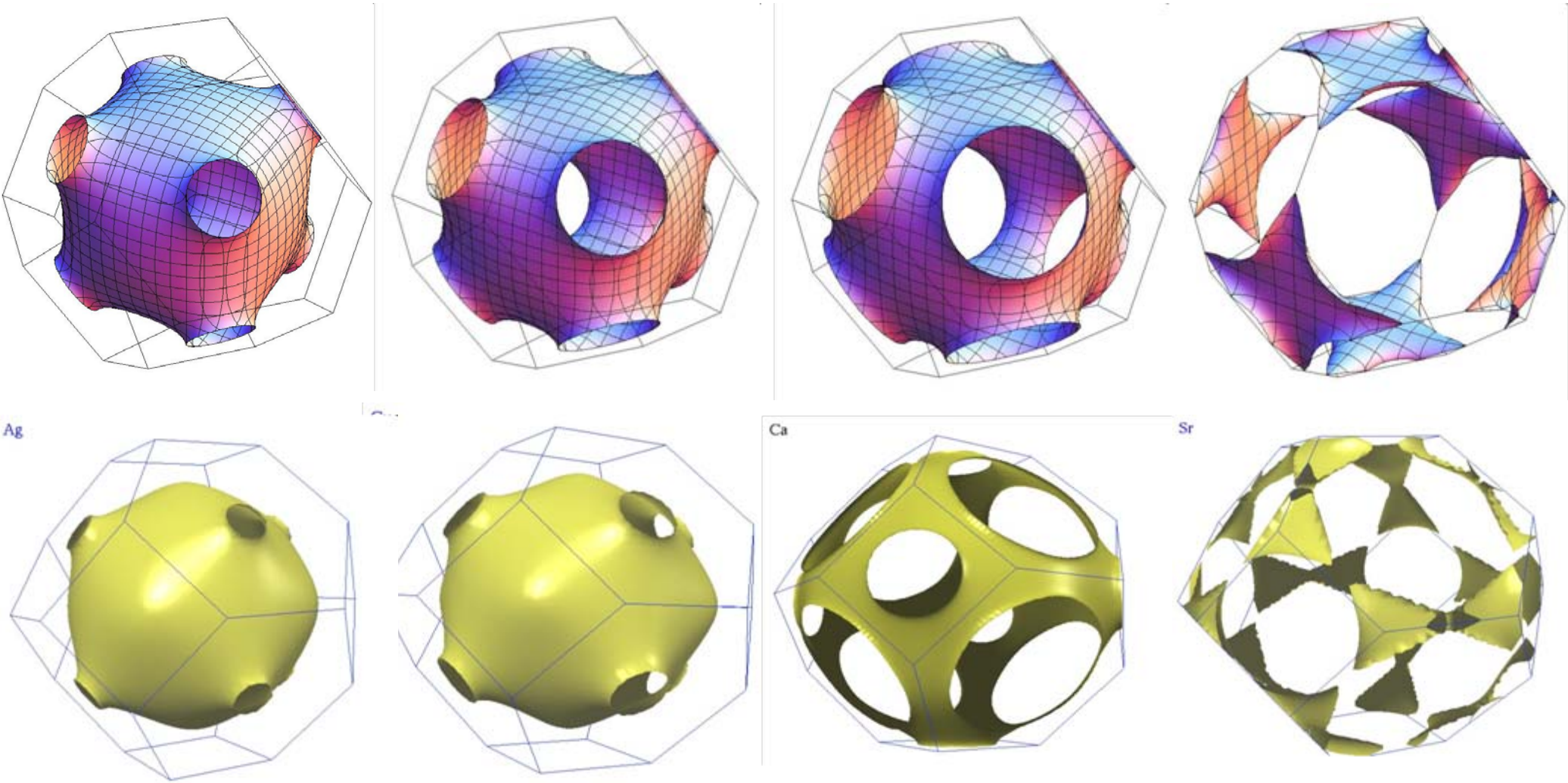
Tight binding, fcc





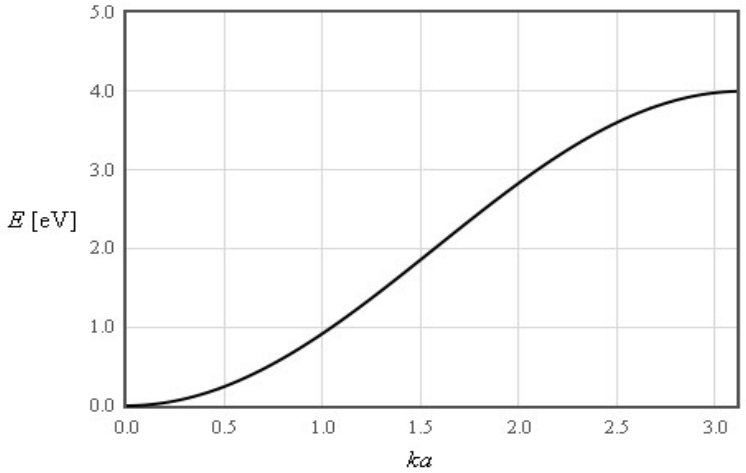
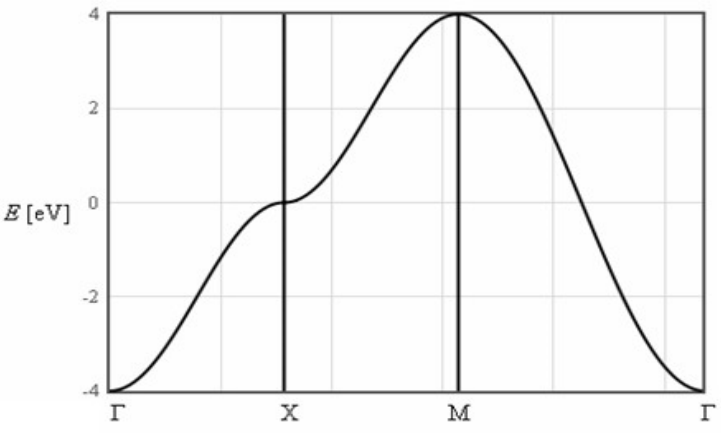
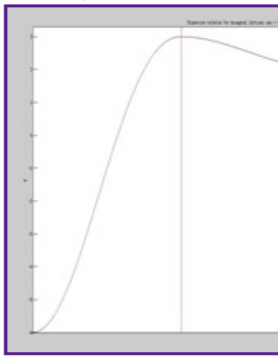
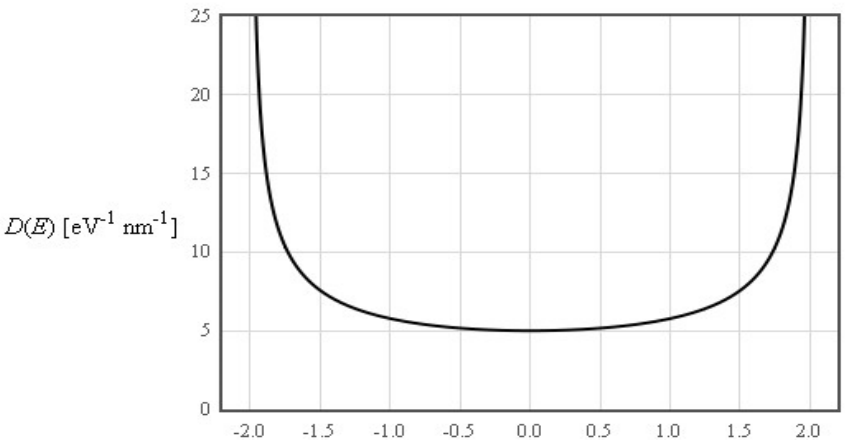
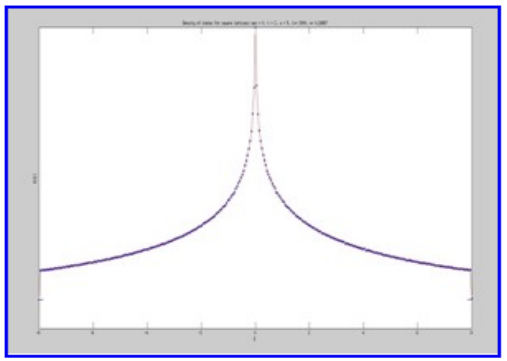
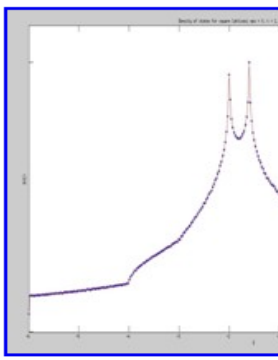
Christian Gruber, 2008

Tight binding, fcc



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

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

	Linear Chain	2-D square lattice	2-D hexagon
Dispersion 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)	$E = \varepsilon - 2t\left(\cos(k_x a) + 2\cos\right.$  hexdisp
Density of states	$D(k) = \frac{2}{\pi}$	$D(k) = \frac{k}{\pi}$ m^{-1}	$D(k) = \frac{k}{\pi}$
Density of states	$D(E) = \frac{1}{at\sqrt{1-\left(\frac{\varepsilon - E}{2t}\right)^2}}$ $\mathrm{J}^{-1}\mathrm{m}^{-1}$ 	 squaredos.m	 hexdos

Student Projects

Plot the dispersion relation for hexagonal crystals

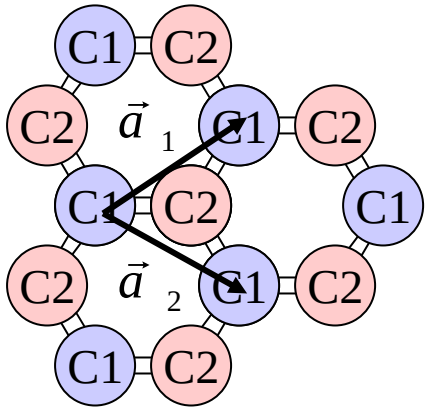
Calculate the density of states for, CNTs, or BN

Draw the missing Fermi surfaces

Calculate the thermodynamic properties based on a calculated DOS

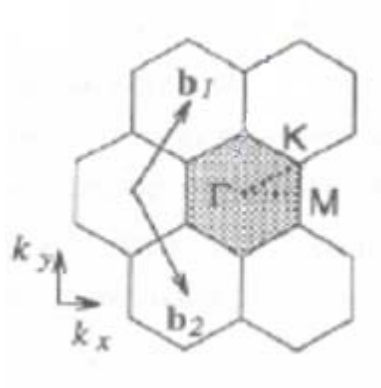
Make a similar table for the plane wave method

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.

Andre Geim

2000 Ig Nobel Prize for levitating a frog with a magnet

The Nobel Prize in Physics 2010
Andre Geim, Konstantin Novoselov

The Nobel Prize in Physics 2010

Nobel Prize Award Ceremony

Andre Geim

Biographical
Nobel Lecture
Banquet Speech
Interview
Nobel Diploma
Photo Gallery
Other Resources

Konstantin Novoselov

Andre Geim

Born: 1958, Sochi, Russia

Affiliation at the time of the award:
University of Manchester,
Manchester, United Kingdom

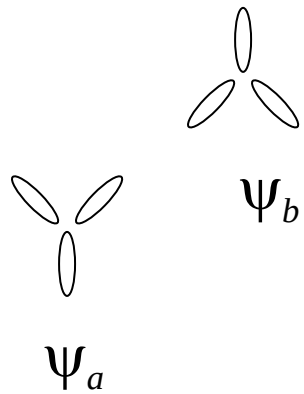
Prize motivation: "for groundbreaking experiments regarding the two-dimensional material graphene"

2 carbon atoms / unit cell

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

$$\psi_k = \sum_{l,m} \exp\left(i\left(l\vec{k}\cdot\vec{a}_1 + m\vec{k}\cdot\vec{a}_2\right)\right)\left(c_a\psi_{p_z a}\left(\vec{r} - l\vec{a}_1 - m\vec{a}_2\right) + c_b\psi_{p_z b}\left(\vec{r} - l\vec{a}_1 - m\vec{a}_2\right)\right)$$

For graphene, the valence orbitals are p_z orbitals



Substitute this wave function into the Schrödinger equation

$$H\psi_k = E\psi_k$$

2 carbon atoms / unit cell

$$\psi_k = \sum_{l,m} \exp\left(i\left(l\vec{k}\cdot\vec{a}_1 + m\vec{k}\cdot\vec{a}_2\right)\right)\left(c_a\psi_{p_z a}\left(\vec{r} - l\vec{a}_1 - m\vec{a}_2\right) + c_b\psi_{p_z b}\left(\vec{r} - l\vec{a}_1 - m\vec{a}_2\right)\right)$$

$$H\psi_k = E\psi_k$$

Multiply by $\psi^*_{p_z a}(\vec{r})$ and integrate

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

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

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

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 $\psi^*_{p_z b}(\vec{r})$ and integrate

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

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

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

$\langle \psi_b | \psi_a \rangle \to 0$

$\langle \psi_b | \psi_b \rangle \to 1$

Write as a matrix equation

Tight binding graphene

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

m sums over the nearest neighbors.

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

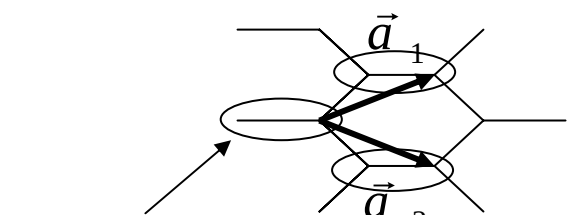
N orbitals / unit cell results in *N* bands

Tight binding graphene

$$\begin{vmatrix} \varepsilon - E & -t\sum_m e^{i\vec{k}\cdot\vec{\rho}_m} \\ -t\sum_m e^{-i\vec{k}\cdot\vec{\rho}_m} & \varepsilon - E \end{vmatrix} = 0$$

$$\sum_m e^{i\vec{k}\cdot\vec{\rho}_m} = \left(1 + \exp\left(i\left(\frac{\sqrt{3}k_x a}{2} + \frac{k_y a}{2}\right)\right)\right) + \exp\left(i\left(\frac{\sqrt{3}k_x a}{2} - \frac{k_y a}{2}\right)\right)$$

$\vec{k}\cdot\vec{a}_1$ $\qquad$ $\vec{k}\cdot\vec{a}_2$



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

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

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

Solve for the dispersion relation

$$\begin{vmatrix} \varepsilon - E & -t\left(1+\exp\left(i\left(\frac{\sqrt{3}k_x a}{2}-\frac{k_y a}{2}\right)\right)+\exp\left(i\left(\frac{\sqrt{3}k_x a}{2}+\frac{k_y a}{2}\right)\right)\right) \\ -t\left(1+\exp\left(-i\left(\frac{\sqrt{3}k_x a}{2}-\frac{k_y a}{2}\right)\right)+\exp\left(-i\left(\frac{\sqrt{3}k_x a}{2}+\frac{k_y a}{2}\right)\right)\right) & \varepsilon - E \end{vmatrix} = 0$$

$$\left(\varepsilon - E\right)^2 - t^2 \begin{pmatrix} 1+\exp\left(i\left(\frac{\sqrt{3}k_x a}{2}-\frac{k_y a}{2}\right)\right)+\exp\left(i\left(\frac{\sqrt{3}k_x a}{2}+\frac{k_y a}{2}\right)\right) \\ +\exp\left(-i\left(\frac{\sqrt{3}k_x a}{2}-\frac{k_y a}{2}\right)\right)+1+\exp\left(-i\left(\frac{\sqrt{3}k_x a}{2}-\frac{k_y a}{2}\right)+i\left(\frac{\sqrt{3}k_x a}{2}+\frac{k_y a}{2}\right)\right) \\ +\exp\left(-i\left(\frac{\sqrt{3}k_x a}{2}+\frac{k_y a}{2}\right)\right)+\exp\left(-i\left(\frac{\sqrt{3}k_x a}{2}+\frac{k_y a}{2}\right)+i\left(\frac{\sqrt{3}k_x a}{2}-\frac{k_y a}{2}\right)\right)+1 \end{pmatrix} = 0$$