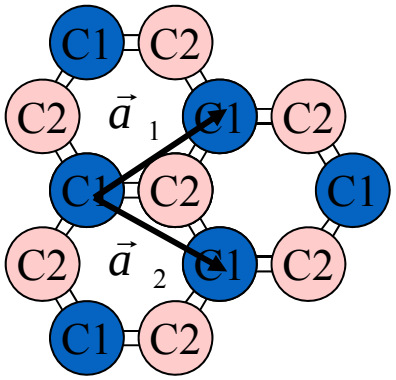
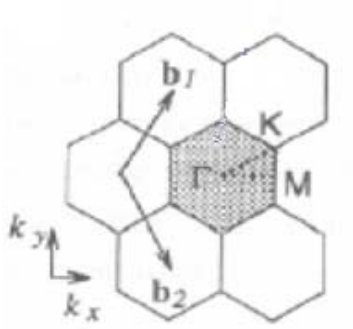
Graphene
Carbon Nanotubes

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

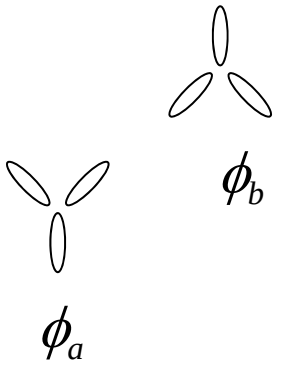
Graphene has an unusual dispersion relation in the vicinity of the Fermi energy.

2 carbon atoms / unit cell

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

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

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

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

$$H\psi_k = E\psi_k$$

Multiply by $\phi^*_{p_z a}(\vec{r})$ 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 $j = 0$, $l = 0$.

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

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

$\langle \phi_b | \phi_a \rangle \to 0$ $\qquad$ $\langle \phi_b | \phi_b \rangle \to 1$

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

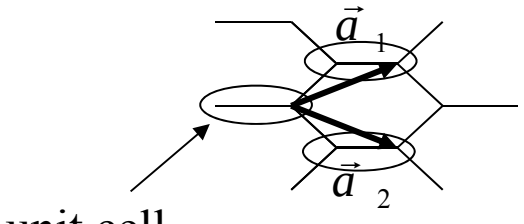
$$\varepsilon = \langle \phi_a | H | \phi_a \rangle$$
$$t = -\langle \phi_a | H | \phi_b \rangle$$

Tight binding graphene

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

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

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



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

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

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

Solve for the dispersion relation

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

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

Graphene dispersion relation

$$(\varepsilon - E)^2 - t^2\left(3 + 2\cos\left(\frac{\sqrt{3}k_x a}{2} - \frac{k_y a}{2}\right) + 2\cos\left(\frac{\sqrt{3}k_x a}{2} + \frac{k_y a}{2}\right) + 2\cos\left(k_y a\right)\right) = 0$$

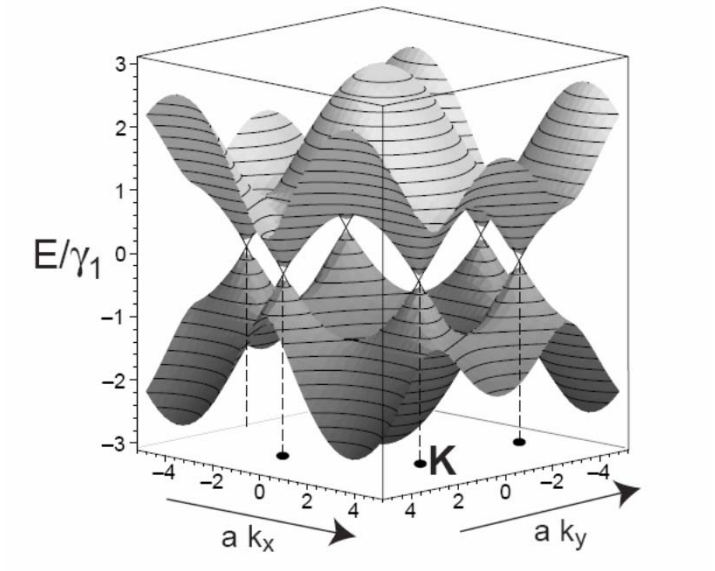
$$\cos(a+b) = \cos a \cos b - \sin a \sin b$$
$$\cos(a-b) = \cos a \cos b + \sin a \sin b$$
$$\cos 2a = 2\cos^2 a - 1$$

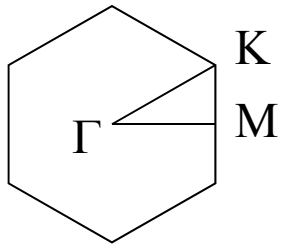
$$(\varepsilon - E)^2 - t^2\left(1 + 4\cos\left(\frac{\sqrt{3}k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right) + 4\cos^2\left(\frac{k_y a}{2}\right)\right) = 0$$

$$E = \varepsilon \pm t\sqrt{1 + 4\cos\left(\frac{\sqrt{3}k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right) + 4\cos^2\left(\frac{k_y a}{2}\right)}$$

Tight binding, graphene

$$E = \varepsilon \pm t\sqrt{1 + 4\cos\left(\frac{\sqrt{3}k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right) + 4\cos^2\left(\frac{k_y a}{2}\right)}$$



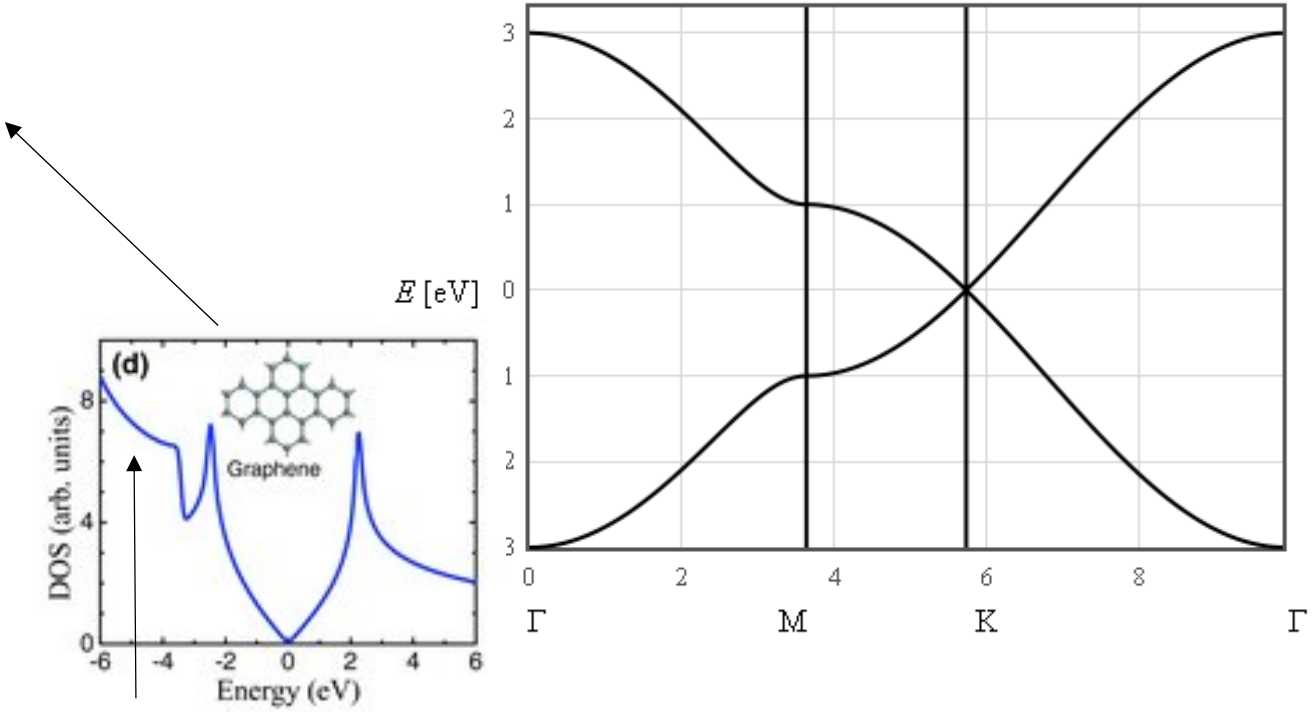


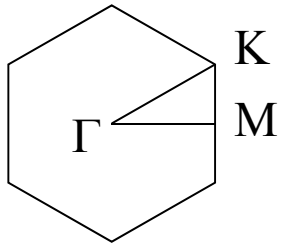
www.physics.umd.edu/courses/Phys732/hdrew/spring07/Schoenenberger%20tutorial%20on%20CNT%20bands.pdf

http://onlinelibrary.wiley.com/doi/10.1002/adfm.201101241/full

Tight binding dispersion relation for graphene

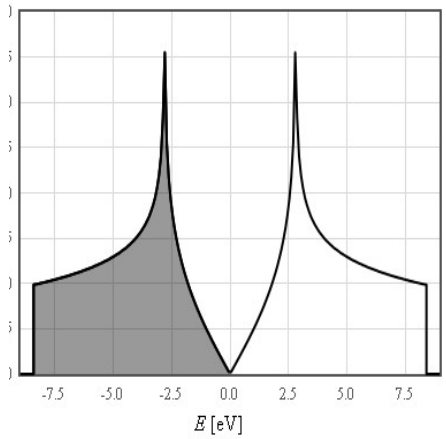
$$E = \varepsilon \pm t\sqrt{1+4\cos\left(\frac{\sqrt{3}k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right)+4\cos^2\left(\frac{k_y a}{2}\right)}$$





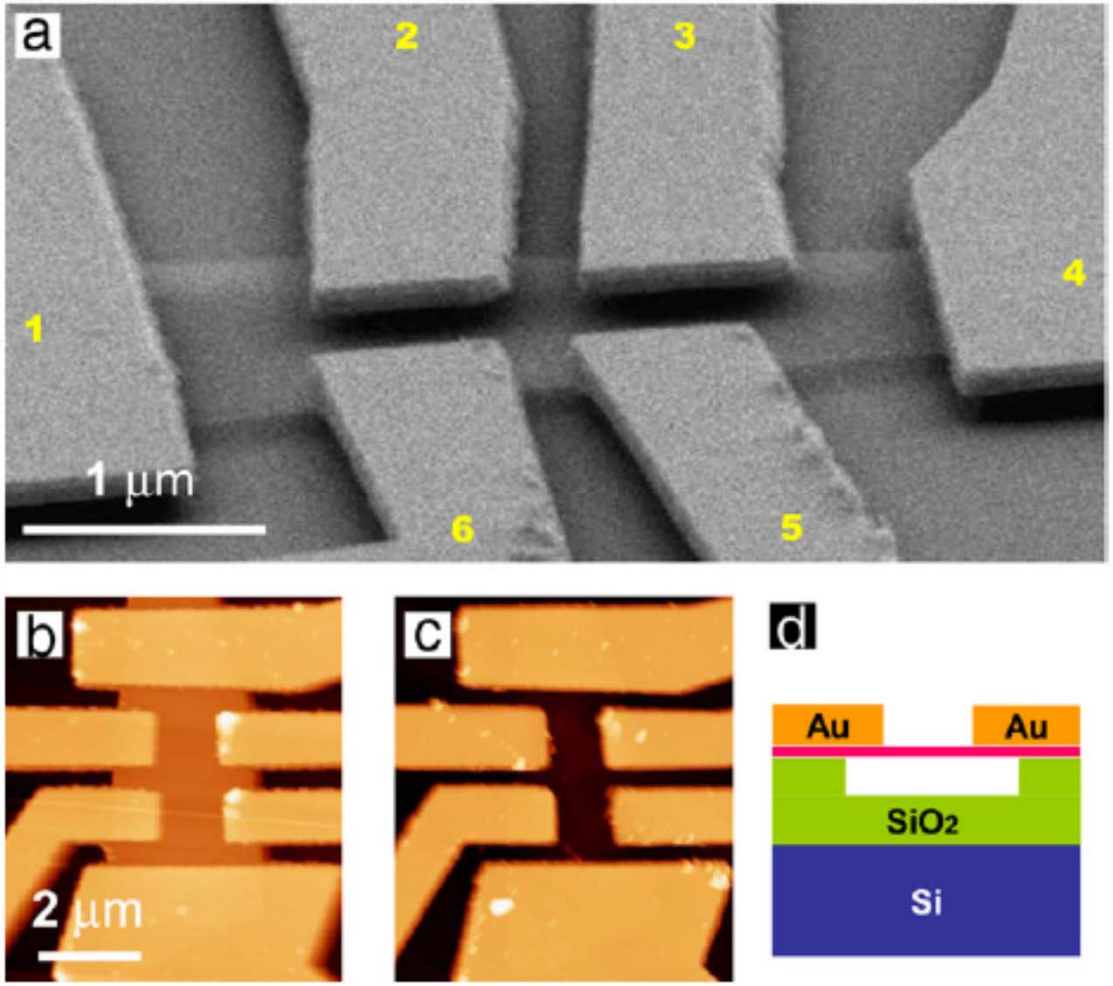
ε = 0 [eV]
t = 2.8 [eV]
Replot E(k)

Another band is included here.



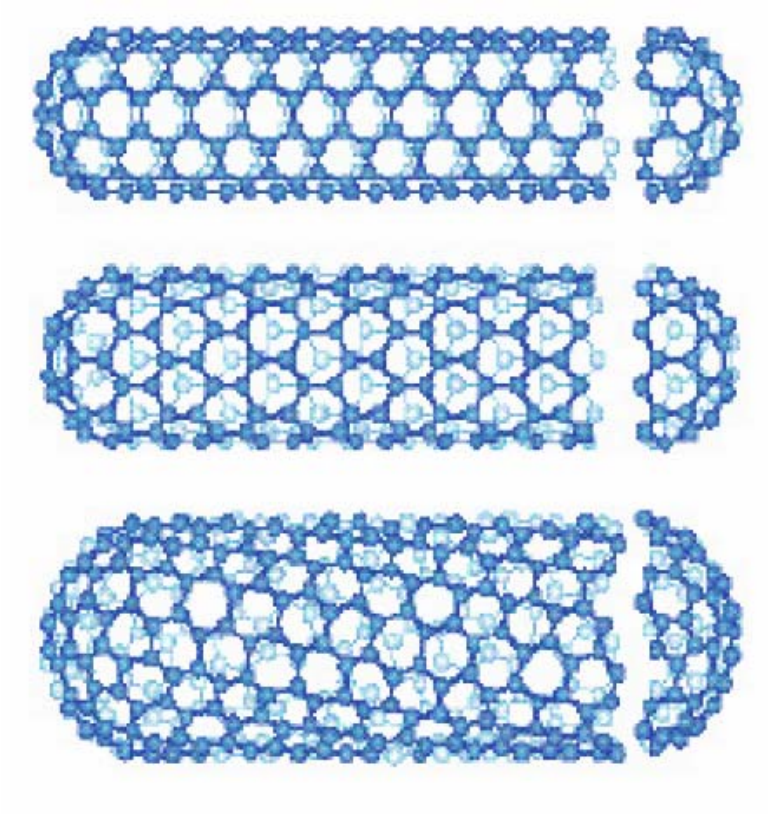
http://lamp.tu-graz.ac.at/~hadley/ss1/bands/tbtable/dispgraphene.html

Graphene



Mobility: 200000 cm^2 /V s suspended, ~20000 cm^2 /V s otherwise

Carbon nanotubes - rolled up graphene



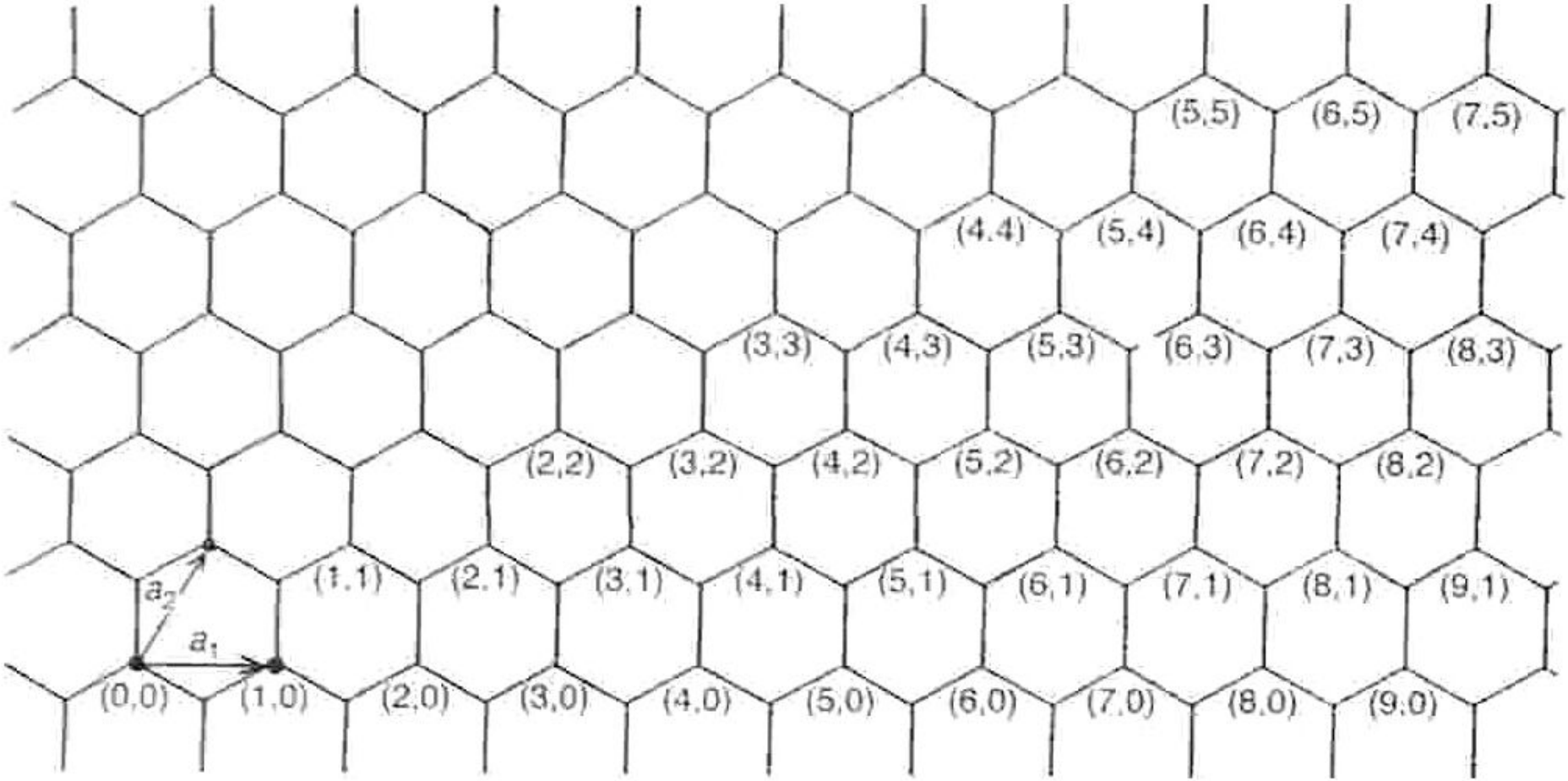
armchair

zig-zag

chiral

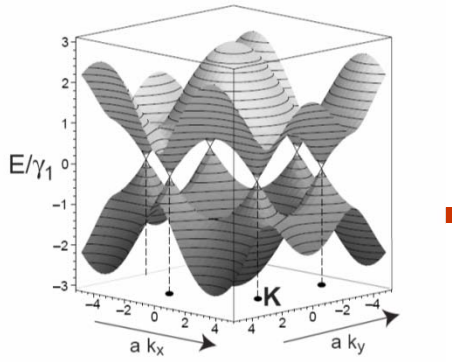
www.physics.umd.edu/courses/Phys732/hdrew/spring07/Schoenenberger%20tutorial%20on%20CNT%20bands.pdf

(*m*,*n*) notation

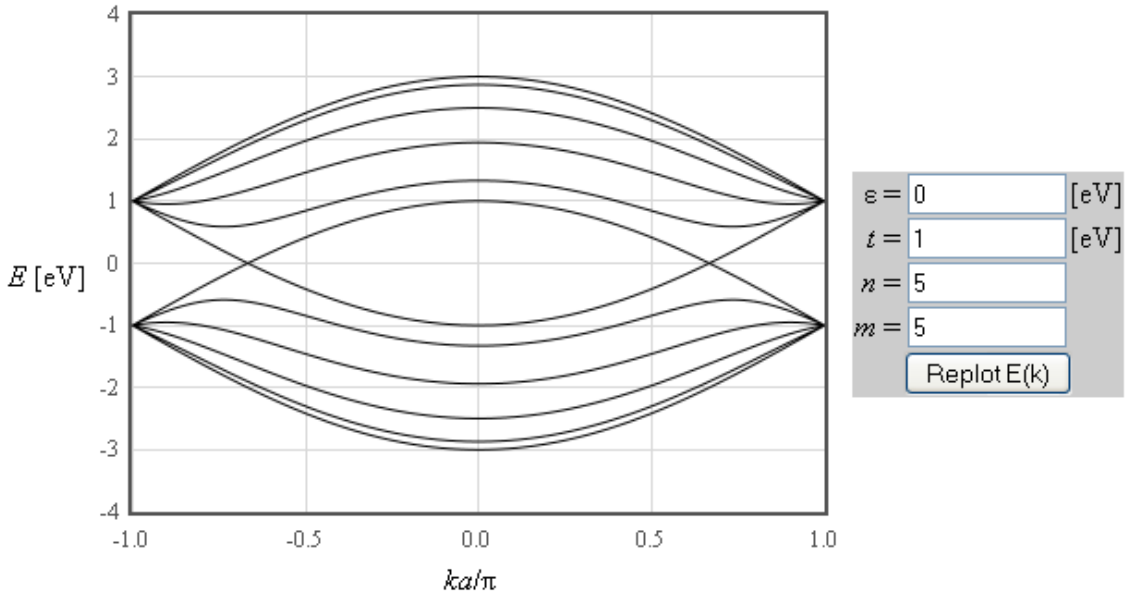


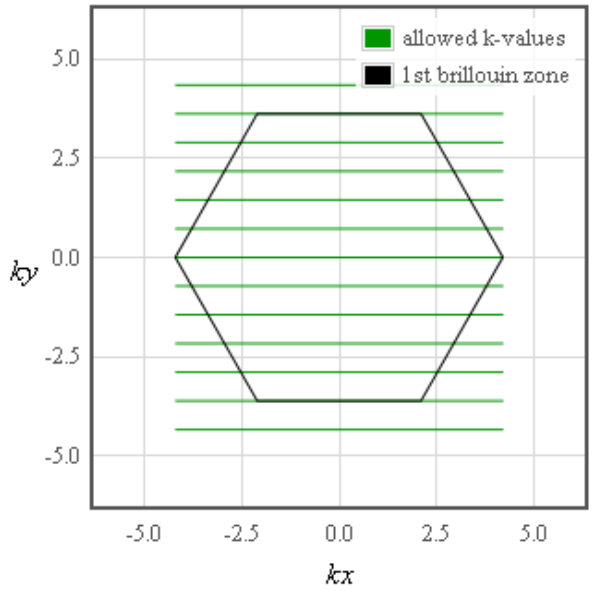
http://www.personal.rdg.ac.uk/~scsharip/tubes.htm

Carbon nanotubes



$$E = \varepsilon \pm t\sqrt{1 + 4\cos\left(\frac{\sqrt{3}k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right) + 4\cos^2\left(\frac{k_y a}{2}\right)}$$





metallic (5,5) armchair tube

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