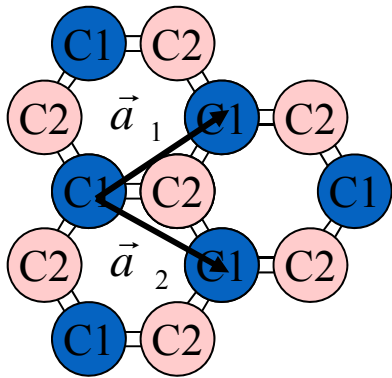


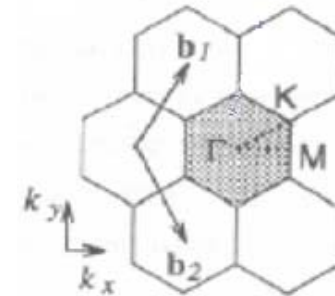
5. Graphene

Oct 17, 2019

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

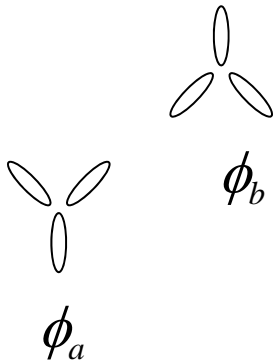
Graphene has an unusual dispersion relation in the vicinity of the Fermi energy.

2 carbon atoms / unit cell

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

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

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

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

$$H\psi_k = E\psi_k$$

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 $j=0, l=0$.

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

0 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

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

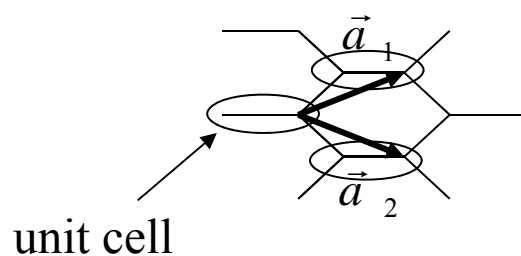
$$t = - \langle \phi_a | H | \phi_b \rangle$$

Tight binding graphene

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

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

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



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

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

There will be two eigen energies for every k .

Solve for the dispersion relation

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

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

Graphene dispersion relation

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

$$\cos(a + b) = \cos a \cos b - \sin a \sin b$$

$$\cos(a - b) = \cos a \cos b + \sin a \sin b$$

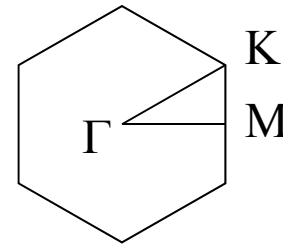
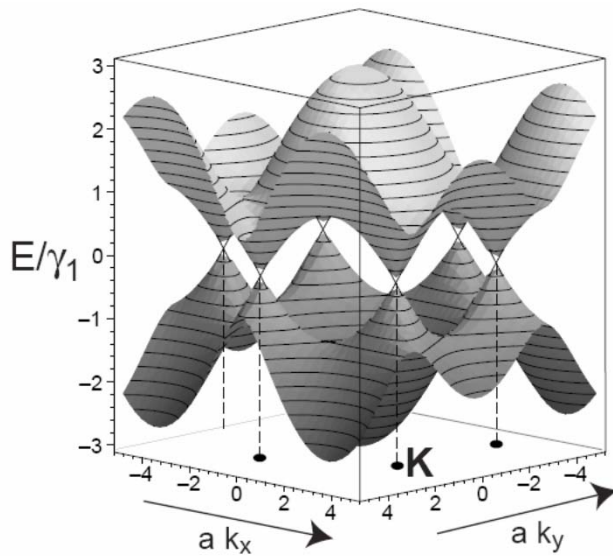
$$\cos 2a = 2 \cos^2 a - 1$$

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

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

Tight binding, graphene

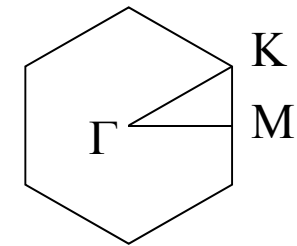
$$E = \varepsilon \pm t \sqrt{1 + 4 \cos\left(\frac{\sqrt{3}k_x a}{2}\right) \cos\left(\frac{k_y a}{2}\right) + 4 \cos^2\left(\frac{k_y a}{2}\right)}$$



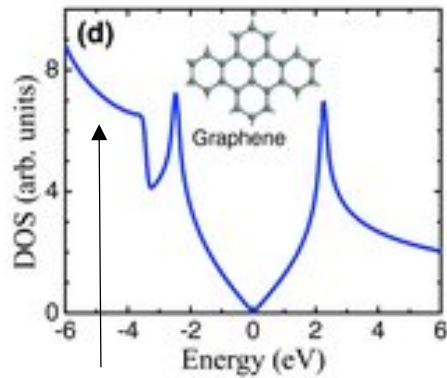
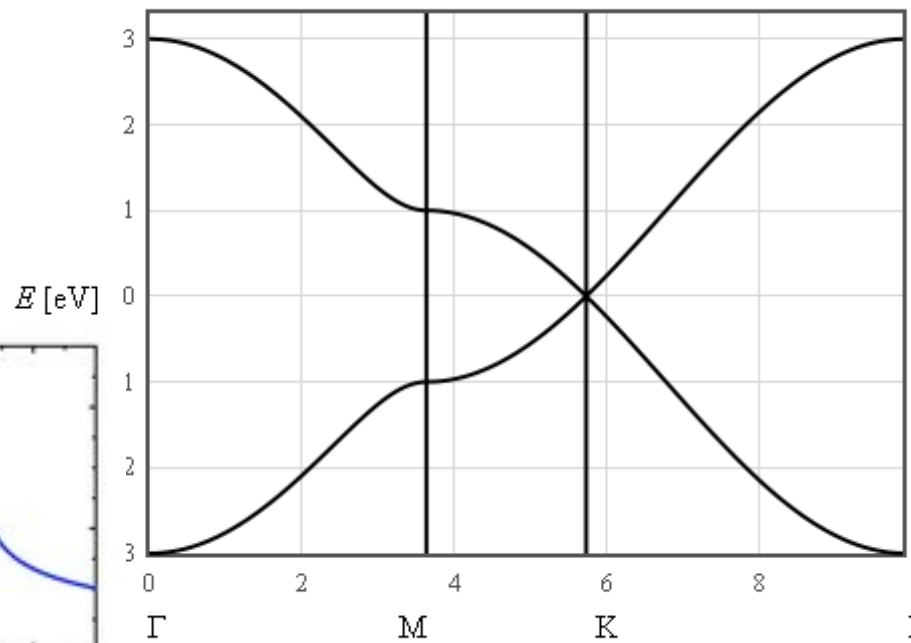
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[www.physics.umd.edu/courses/Phys732/hdrew/spring07/
Schoenenberger%20tutorial%20on%20CNT%20bands.pdf](http://www.physics.umd.edu/courses/Phys732/hdrew/spring07/Schoenenberger%20tutorial%20on%20CNT%20bands.pdf)

Tight binding dispersion relation for graphene

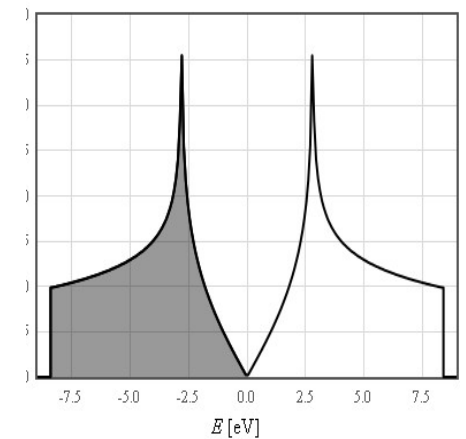
$$E = \varepsilon \pm t \sqrt{1 + 4 \cos\left(\frac{\sqrt{3}k_x a}{2}\right) \cos\left(\frac{k_y a}{2}\right) + 4 \cos^2\left(\frac{k_y a}{2}\right)}$$



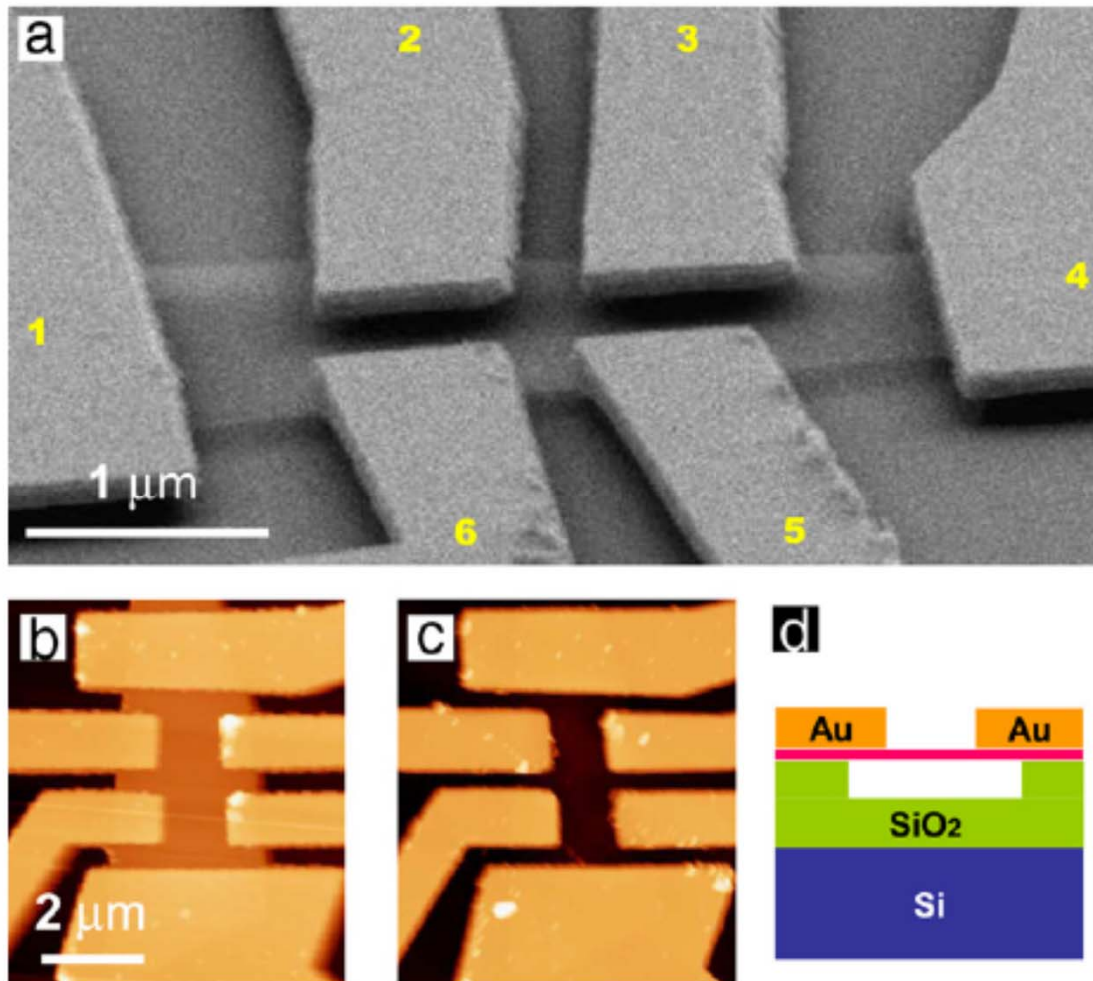
$\varepsilon = 0$ [eV]
 $t = 2.8$ [eV]
Replot E(k)



Another band is included here.

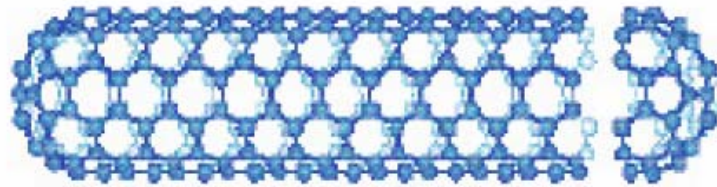


Graphene

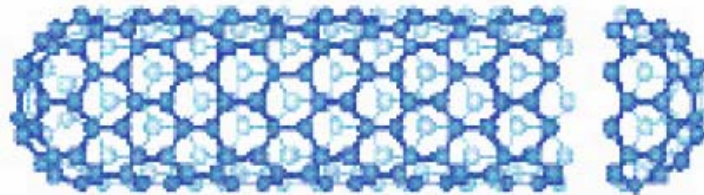


Mobility: 200000 $\text{cm}^2 / \text{V s}$ suspended, $\sim 20000 \text{ cm}^2 / \text{V s}$ otherwise

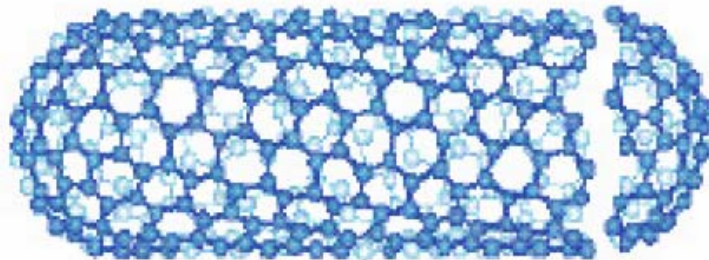
Carbon nanotubes - rolled up graphene



armchair



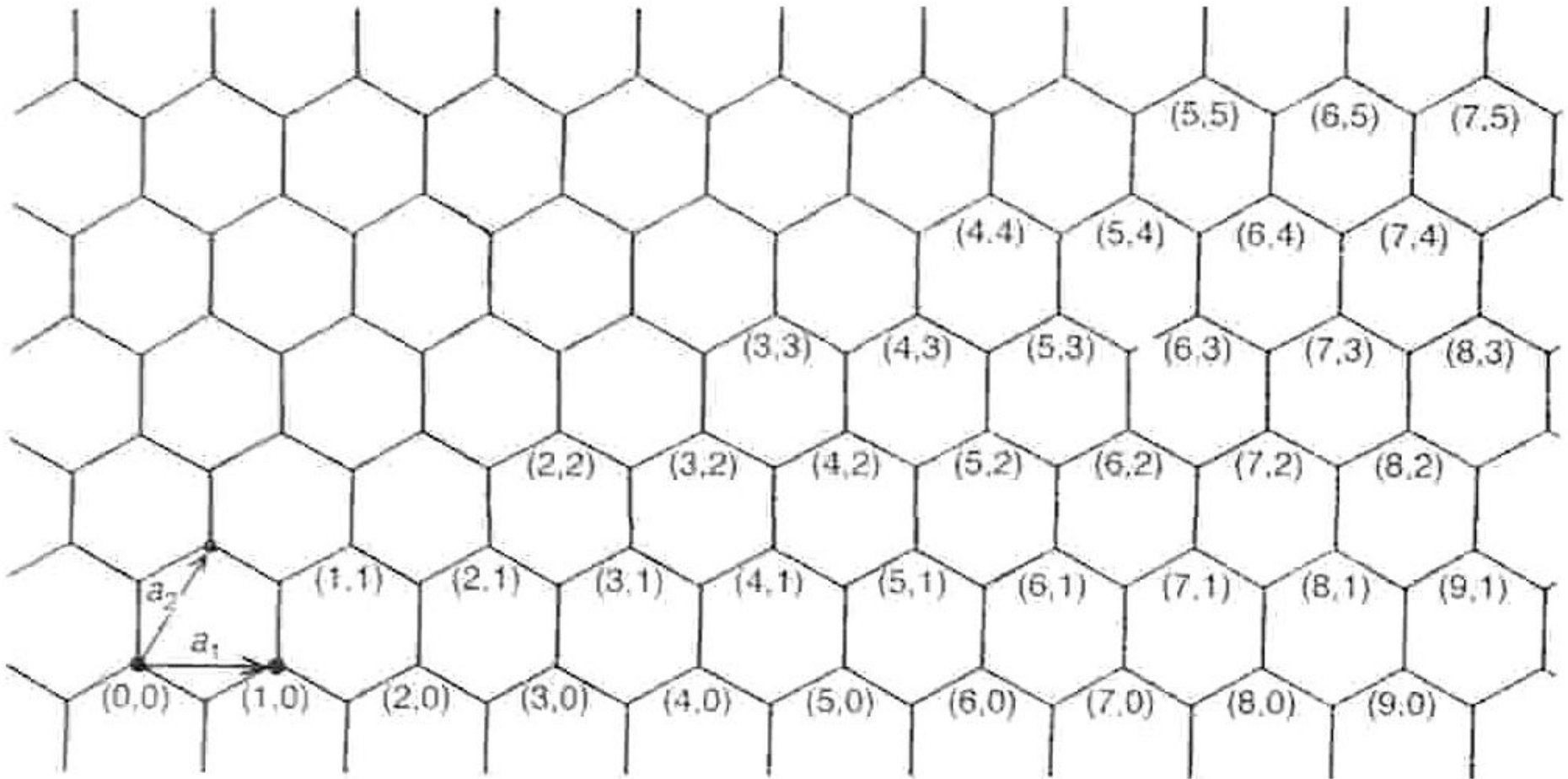
zig-zag



chiral

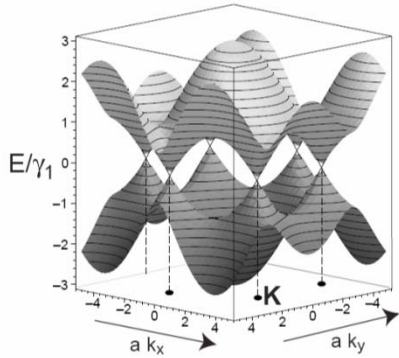
[www.physics.umd.edu/courses/Phys732/hdrew/spring07/
Schoenenberger%20tutorial%20on%20CNT%20bands.pdf](http://www.physics.umd.edu/courses/Phys732/hdrew/spring07/Schoenenberger%20tutorial%20on%20CNT%20bands.pdf)

(m,n) notation

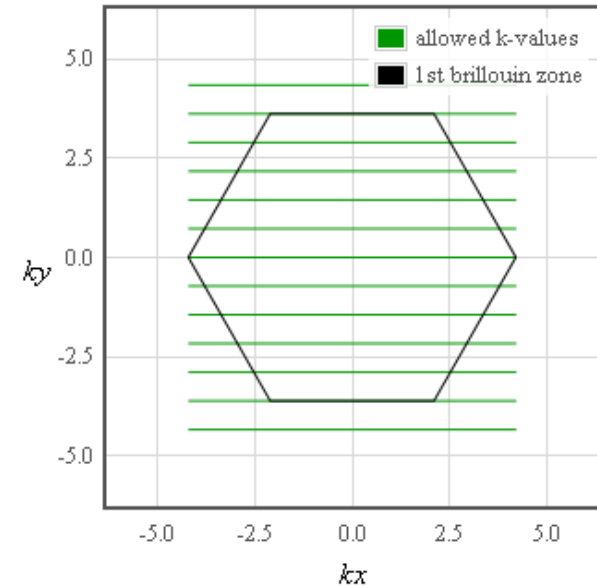
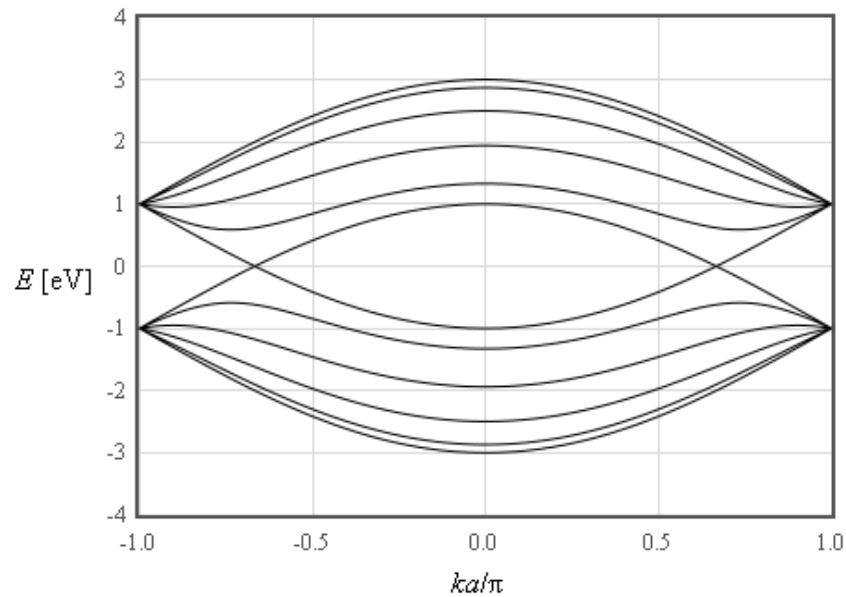


<http://www.personal.rdg.ac.uk/~scsharip/tubes.htm>

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>