Single-Wall Carbon Nanotubes: Lattice, e^- bands, and Transport

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Lattice Structure

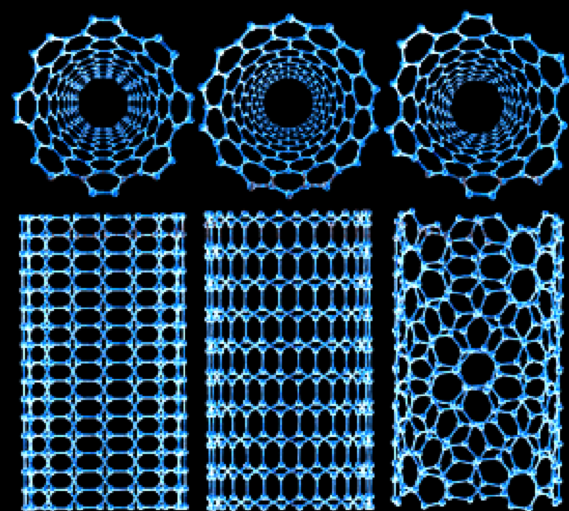
A CNT is rolled strip of Graphene
- geometry defined by a mapping of unit cell onto graphene lattice.
- mapping is a function of two integers, n, m
- defines the "chiral vector"

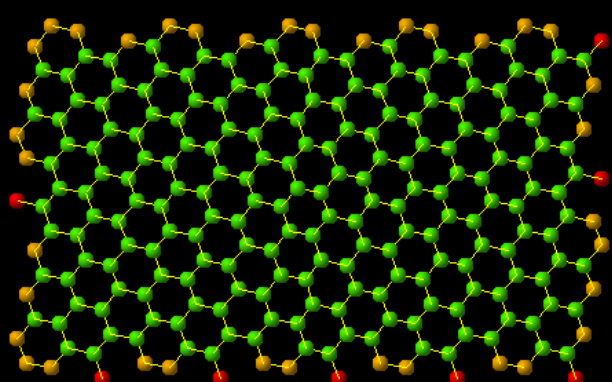
$$\boldsymbol{C}_h = n\boldsymbol{a}_1 + m\boldsymbol{a}_2$$

and "translational vector"

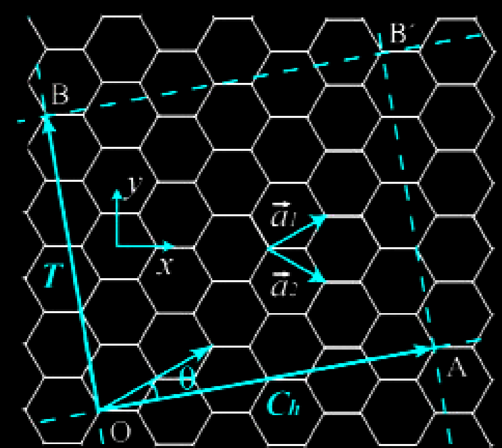
$$\boldsymbol{T} = t_1(n,m)\boldsymbol{a}_1 + t_2(n,m)\boldsymbol{a}_2$$

armchair	zig-zag	chiral
(n,n)	$(n,0)$	(n,m)





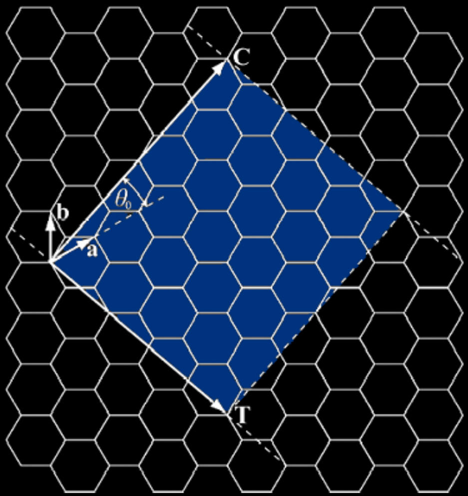
http://www.photon.t.u-tokyo.ac.jp/~maruyama/agallery/agallery.html



http://www.ks.uiuc.edu/Research/nanotube/

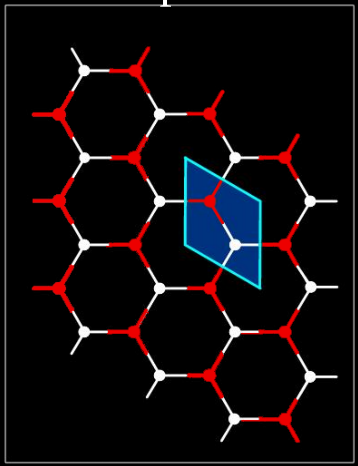
Reciprocal Lattice

CNT



http://spie.org/x15004.xml?ArticleID=x15004

Graphene



http://www.scitizen.com/stories/NanoSciences/2007/11/
A-Theorist-s-Pencil-and-One-Layer-of-Carbon-Atoms-Graphene/

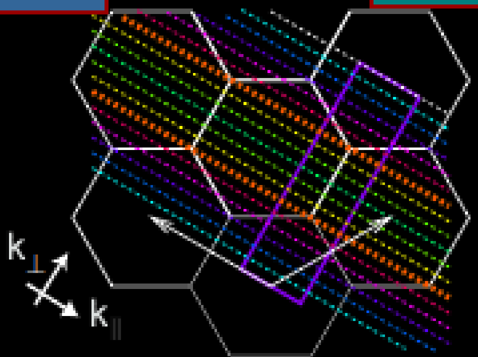
Boundary Conditions

$$\Psi(\boldsymbol{r} + p\boldsymbol{T}) = \Psi(\boldsymbol{r})$$
$$\Psi(\boldsymbol{r} + \boldsymbol{C}_h) = \Psi(\boldsymbol{r})$$

$$\Psi(\boldsymbol{r} + p\boldsymbol{a}_1) = \Psi(\boldsymbol{r})$$
$$\Psi(\boldsymbol{r} + q\boldsymbol{a}_2) = \Psi(\boldsymbol{r})$$

$p, q \in \mathcal{Z}$

$$\boldsymbol{k} = x_1\boldsymbol{k}_\perp + x_2\boldsymbol{k}_{||}$$
$$x_1 = 0, 1, \ldots N-1$$
$$x_2 \in [0, 1]$$

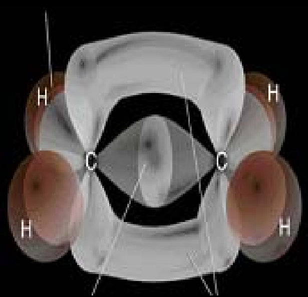


$\boldsymbol{k}$-space

(Grove-Rasmussen 2006)

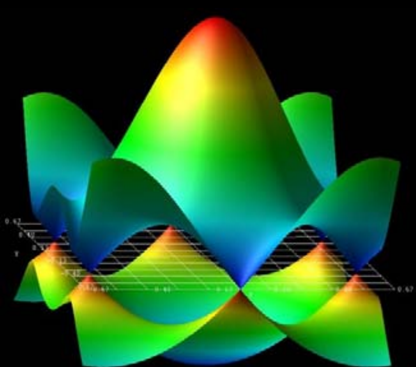
$$\boldsymbol{k} = x_1\boldsymbol{b}_1 + x_2\boldsymbol{b}_2$$
$$x_1 \in [0, 1]$$
$$x_2 \in [0, 1]$$

Tight Binding Energy Bands



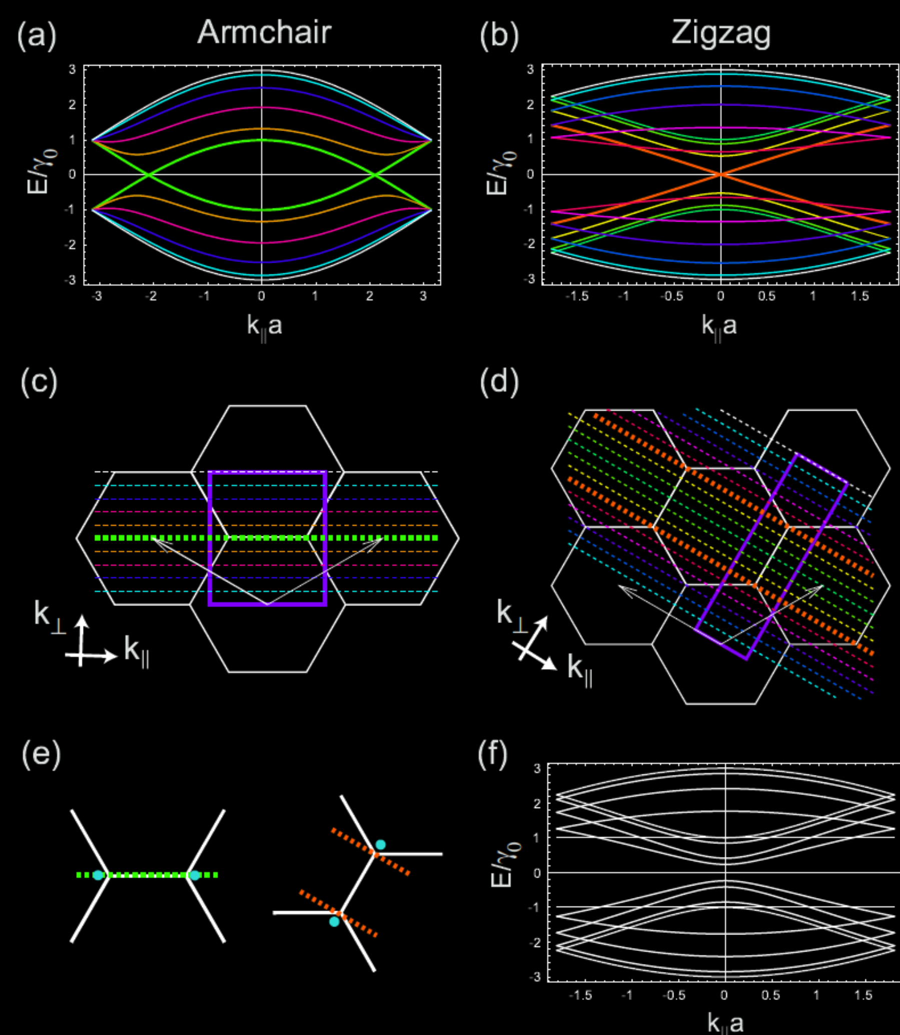
Ethylene molecule displaying sp^2 hybridization

http://www.science.uwaterloo.ca/~cchieh/cact/c120/hybridcarbon.html



graphene tight binding for π bands

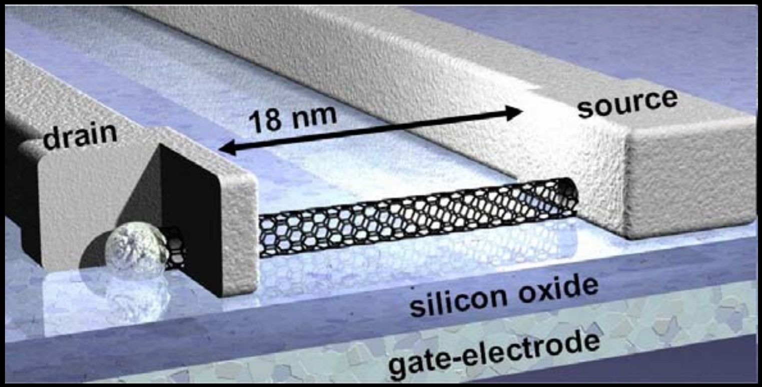
http://www.nextnano.de/nextnano3/tutorial/1Dtutorial_TightBinding_graphene.htm



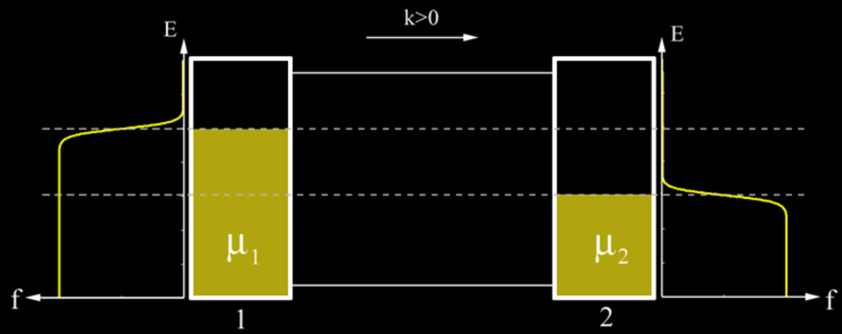
Armchair and Zigzag SWCNT band strucure

Grove-Rasmussen 2006

Ballistic Transport, $L_m, L_\phi > L$



http://nanopedia.case.edu/image/Infineon-nanotube.jpg



Landauer Formula (ignore reflections at contacts)

$$I = \frac{2e}{h}\int_{-\infty}^{\infty}[f(\mathcal{E}-\mu_1) - f(\mathcal{E}-\mu_2)]M(\mathcal{E})\mathcal{T}(\mathcal{E})d\mathcal{E}$$

Spin degeneracy

# of available electrons for transport

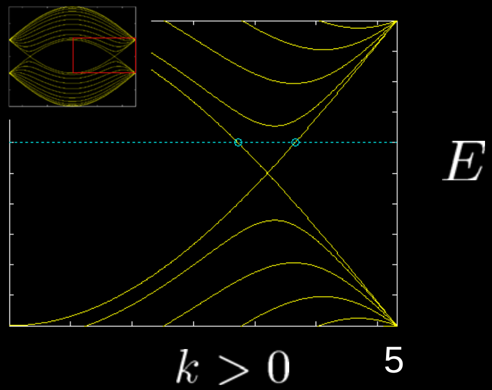
# of channels

Transmission Probability

For T=0, M=const, $\mathcal{T}$ =const

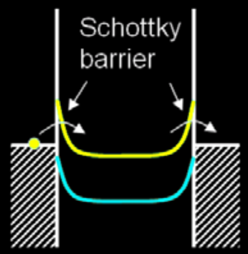
$$I = \boxed{\frac{2e^2}{h}M\mathcal{T}}\frac{\mu_1-\mu_2}{e}$$

Quantized conductance $\leq \frac{4e^2}{h}$ (near fermi energy)

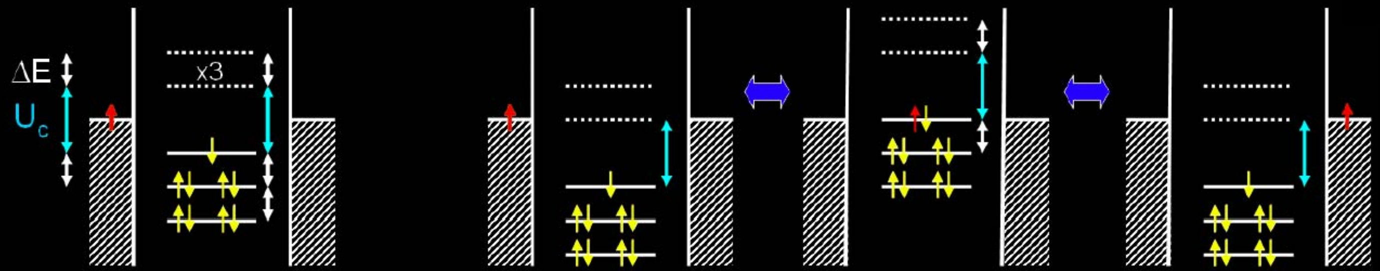


Coulomb Blockade

For Large Schottky barrier, Nanotube becomes a weakly coupled quantum dot.



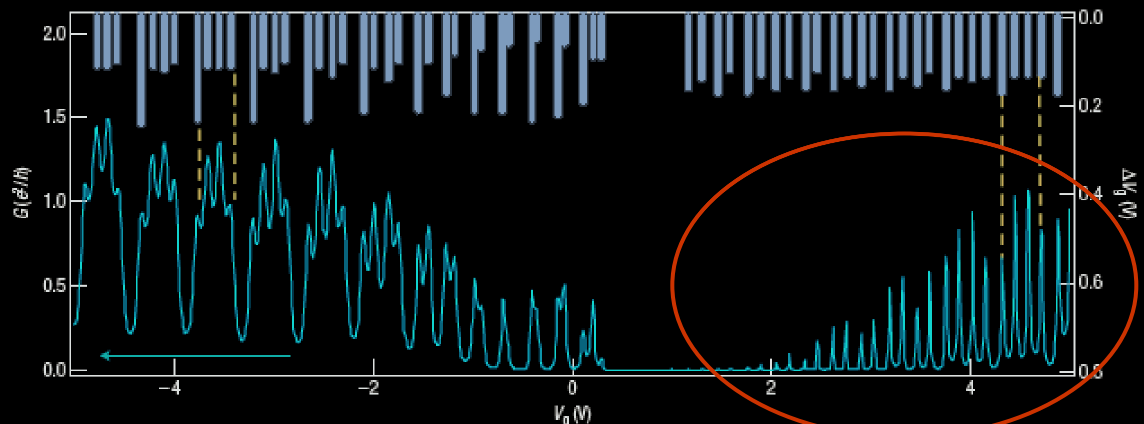
Tunneling carriers must pay additional charging energy, U_c



Grove-Rasmussen 2006

Blockade

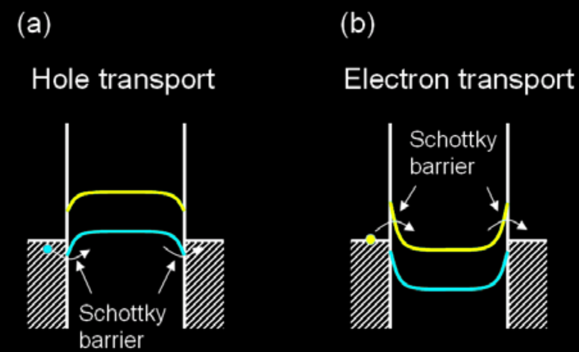
Single electron transport



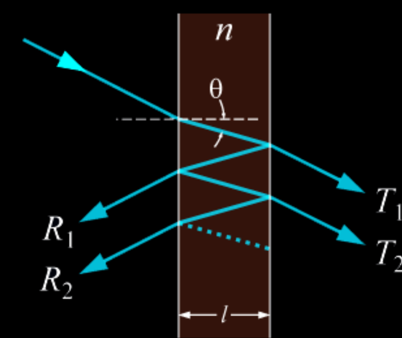
Cao et.al. 2005

Conductance oscillations due to blockade

Fabry-Perot Interference

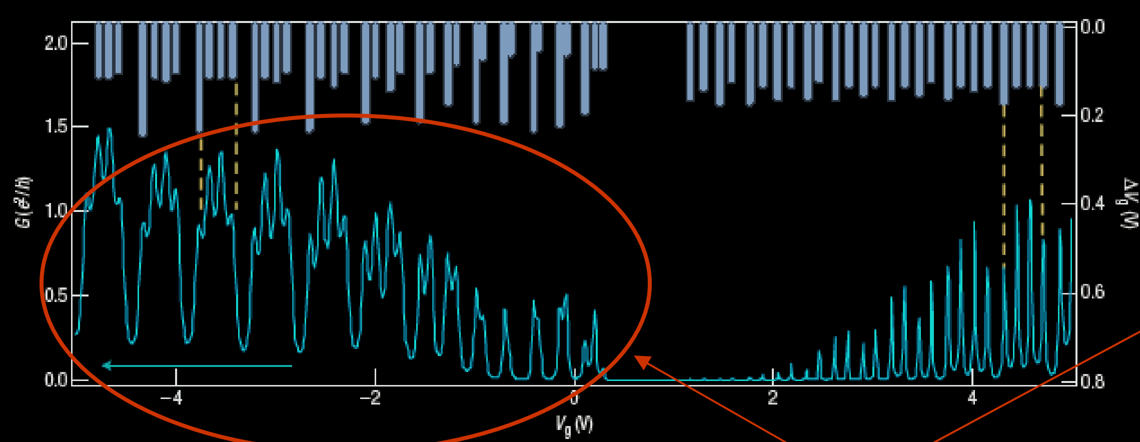


Small Schottky barrier allows for transport with reflections at contacts.

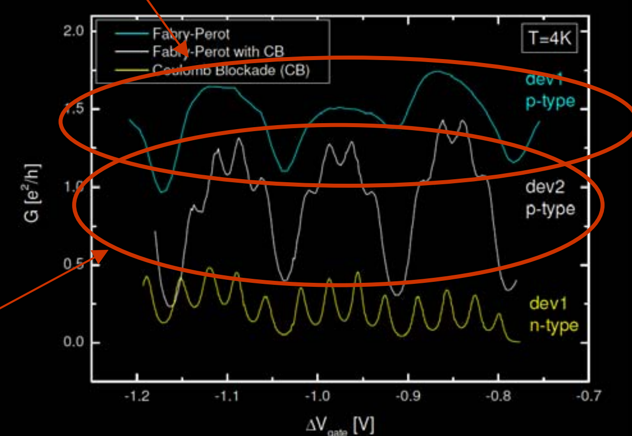


http://en.wikipedia.org/wiki/Fabry-P%C3%A9rot_interferometer

Fabry-Perot conductance oscillations



Cao et.al. 2005



Grove-Rasmussen 2006

Fabry-Perot and Coulomb blockade together

Thank you.

Questions?