

# MUNDO MARAVILHOSO DO CARBONO NANOCIÊNCIA



INSTITUTO DE FÍSICA  

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Universidade Federal Fluminense

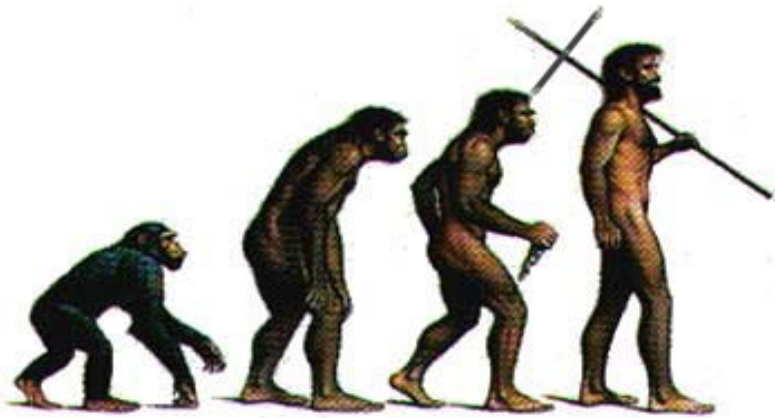
**Andrea Latgé**  
**UFF/IF**



# SISTEMAS NANOESTRUTURADOS



[www.nano.if.uff.br](http://www.nano.if.uff.br)



# Avanços Tecnológicos e Científicos

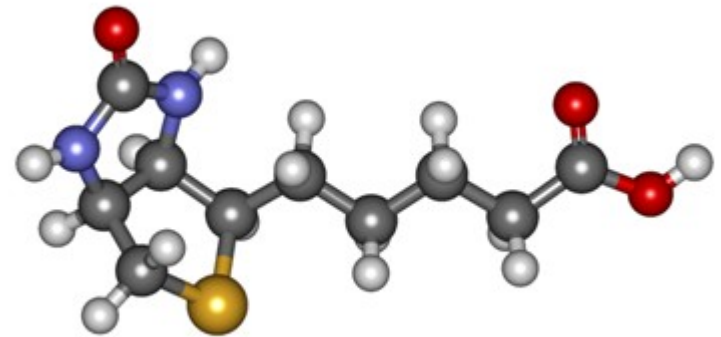
## NANOCIÊNCIA & NANOTECNOLOGIA





# FÍSICA – NANOCIÊNCIA – NANOTECNOLOGIA

- O que é nanociência?





## ❖ O que é **NANOciência**?

Nano do Grego “nanos” (ou Latin “nanus”), significa anão

Nano  $10^{-9}$  –nanômetro, da escala do diâmetro atômico (o cabelo humano tem uma espessura de cerca de 100 nm)

➡ Nanociência é o estudo dos átomos, moléculas, e objetos cujos tamanhos estão na escala **dos nm's ( 1 - 100 nm)**.

## ❖ Por que o estudo da **NANOciência** é diferente dos problemas em escalas maiores?

A **FÍSICA** é diferente na escala nanométrica. Propriedades que não são vistas numa escala macroscópica se tornam importantes – “quantum mechanical and thermodynamic”. Se trabalha com átomos individuais e moléculas.

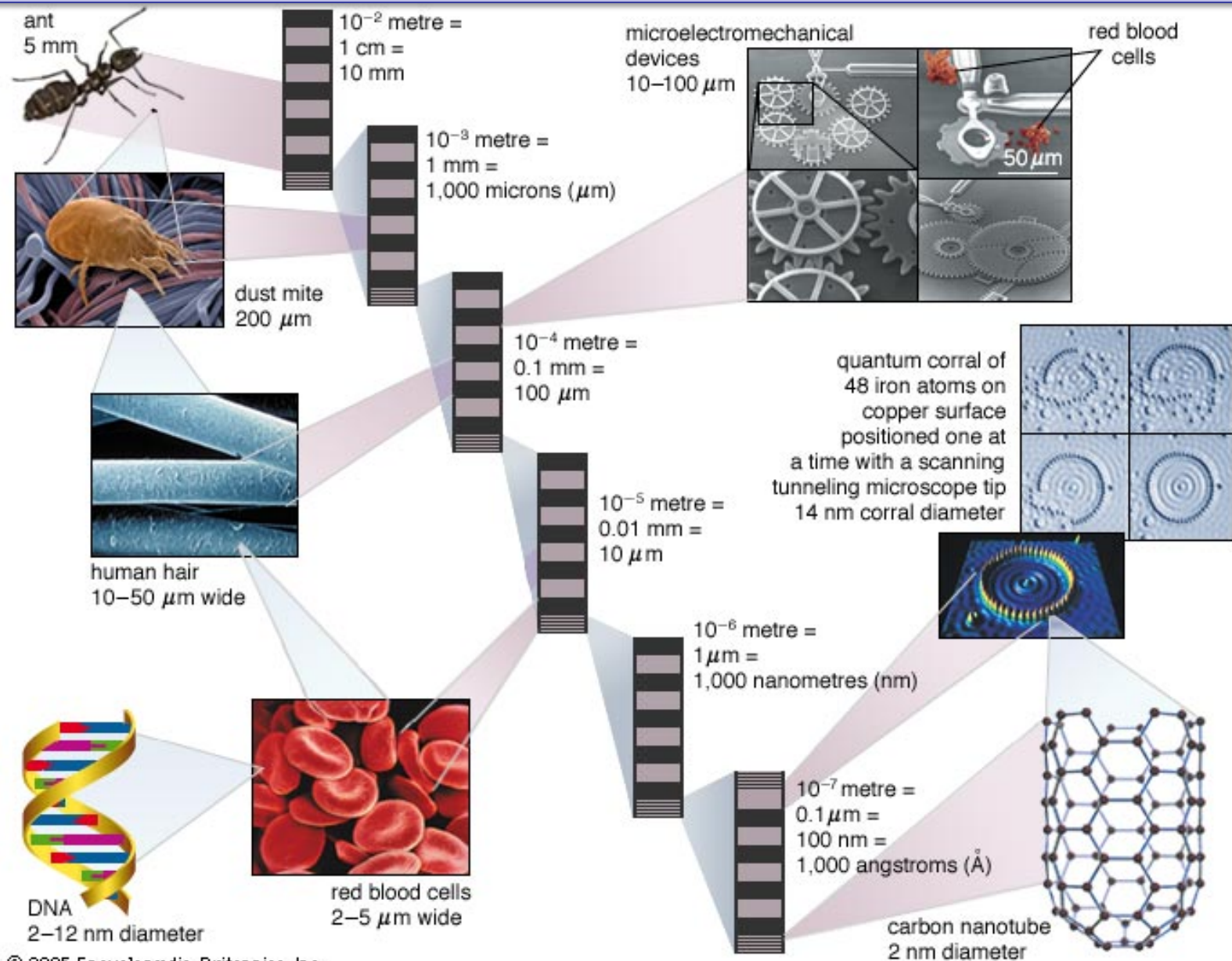
Moléculas individuais - agrupar em formas bem determinadas para produzir novos materiais com características novas e interessantes.

## ❖ Pq **NANOCIÊNCIA** se tornou um grande campo de interesses?

Muitas razões: Disponibilidade de novos instrumentos capazes de “**ver**” e “**tocar**” nesta escala.



# VARIANDO TAMANHOS.....DO METRO (m) AO ANGSTRON (Å)



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# Manipular átomos é muito difícil devido as suas dimensões

- Submúltiplos do metro (m)

$$10^{-3} \text{ m} = 1 \text{ mm}$$

(milímetro)  
"macromundo"



Formiga

4 – 5 mm



Cabeça de um prego

1 – 2 mm

$$10^{-6} \text{ m} = 1 \mu\text{m}$$

(microns)  
"micromundo"



Tecidos celulares

2 – 5  $\mu\text{m}$

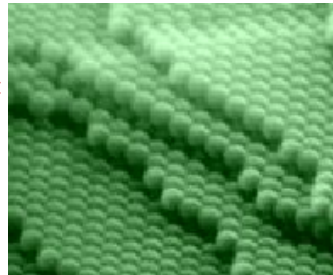


Microengrenagens

10 – 100  $\mu\text{m}$

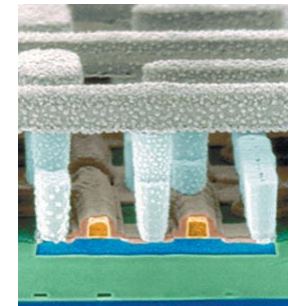
$$10^{-9} \text{ m} = 1 \text{ nm}$$

(nano)  
"nanomundo"\*



Distância entre átomos de silício

0.4 – 0.5 nm



Nanochips

10 – 100 nm







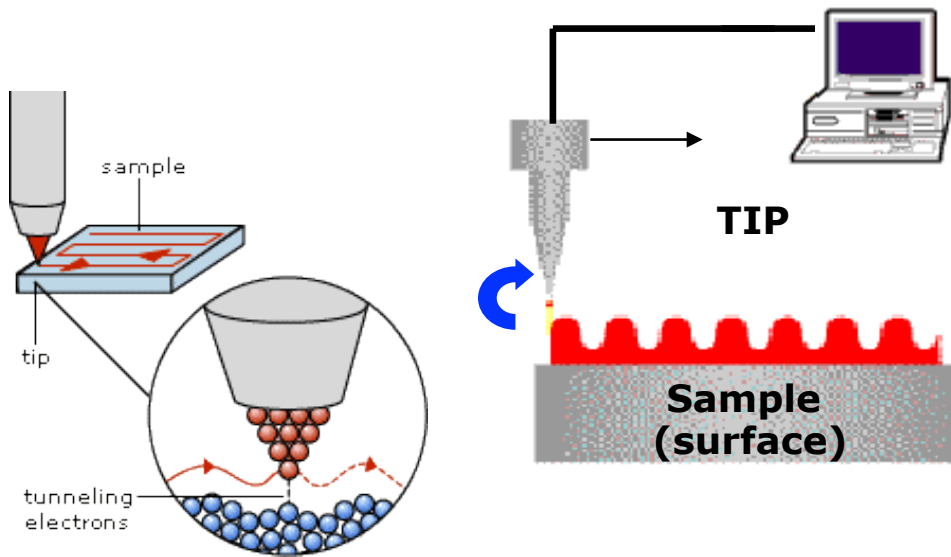
Um dos feitos mais importantes para **o desenvolvimento da N&N** - invenção em 1981 do microscópio de varredura por tunelamento eletrônico. A concepção deste microscópio é bastante simples (funcionamento dos antigos toca-discos).

Uma agulha extremamente fina, cuja ponta é constituída de alguns poucos átomos ou até mesmo de um único átomo, "tateia" uma superfície sem nela tocar, dela afastada de menos de um nanometro.

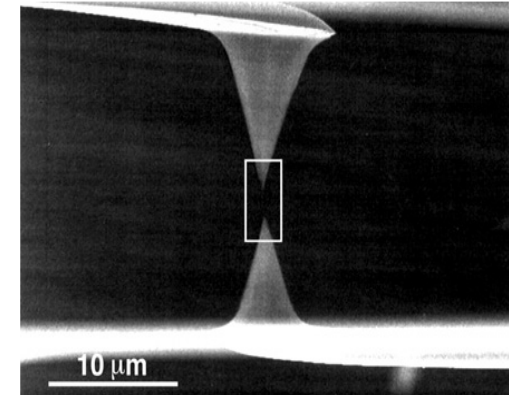
Durante a **varredura da agulha**, elétrons tunelam (tunelamento é uma forma de movimento de origem quântica que ocorre na escala atômica) da agulha para a superfície e com base nessa corrente de tunelamento um computador constrói uma imagem extremamente ampliada da superfície, na qual ficam visíveis os seus átomos. Dessa forma, pela primeira vez o relevo atômico da superfície de uma estrutura pôde ser visto e investigado. Ele deu origem a uma família de instrumentos de visualização e manipulação na escala atômica, coletivamente denominados microssondas eletrônicas de varredura. Em um sentido figurado, eles podem operar como pinças capazes de manipular átomos e moléculas.



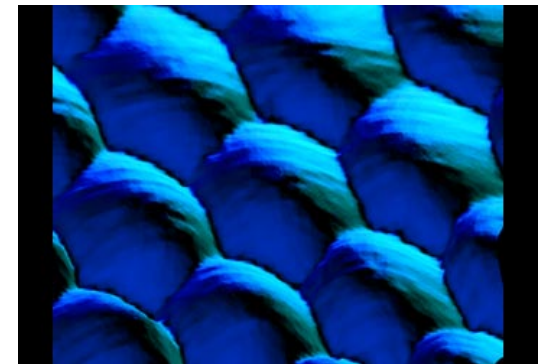
# PROGRESSO DEVIDO AOS AVANÇOS TECNOLÓGICOS EXPERIMENTAIS

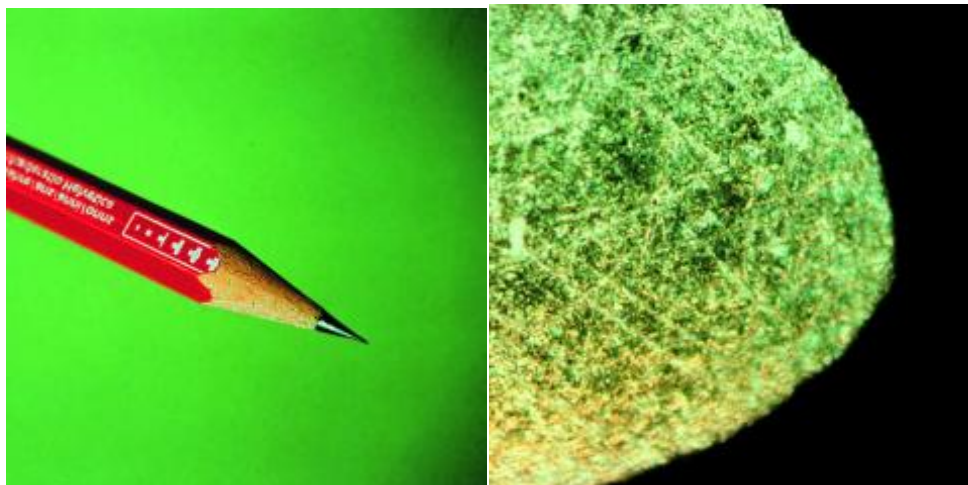


***Scanning Tunneling  
Microscope - STM***



**Blue Platinum**  
The surface of Platinum.



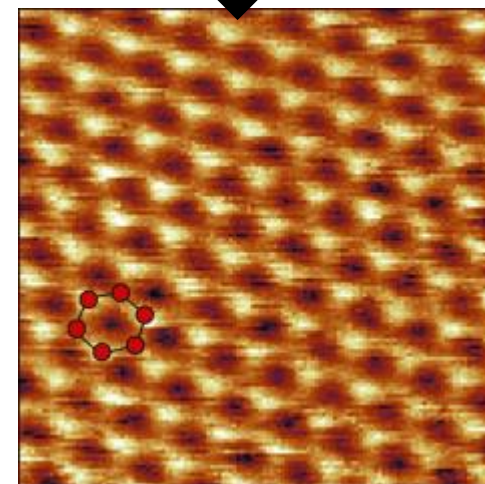
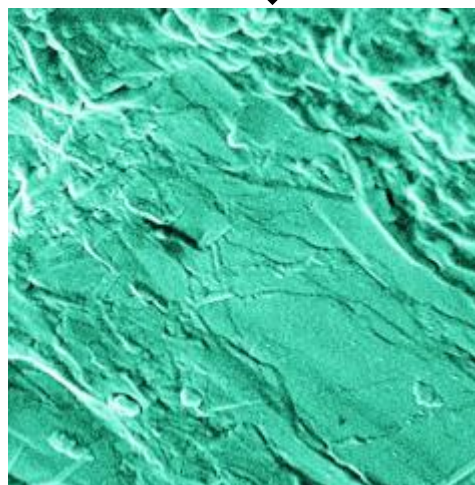


**Grafite a olho nú**

**Grafite por  
microscópio de luz**

**Grafite microscópio  
eletrônico**

**Grafite por microscopia  
de varredura**



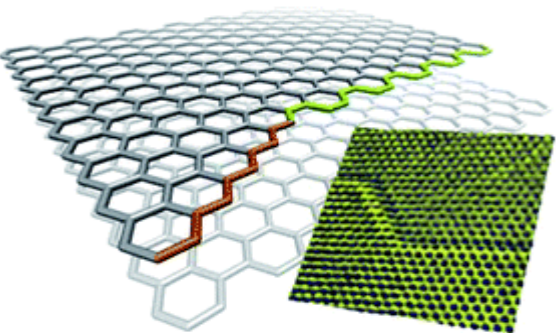


**N&N** - criação de novas **moléculas** com arquiteturas especiais. Invenção e produção de moléculas cuja arquitetura faça com que elas se auto-organizem em estruturas maiores (como moléculas biológicas).

Possibilidades futuras: computadores moleculares muito mais poderosos, catalisadores nanométricos mais diversificados e eficientes, materiais avançados para próteses, e até anticorpos sintéticos capazes de encontrar e destruir vírus ou células cancerígenas onde eles se encontrem no corpo.

**Farmacologia** pode obter avanços revolucionários advindos da **N&N**. Os princípios ativos das drogas podem ser agregados à superfície ou encapsulados no interior de macromoléculas projetadas para serem absorvidas por órgãos específicos do corpo, ou por órgãos afetados por determinadas doenças, onde finalmente liberarão a droga.

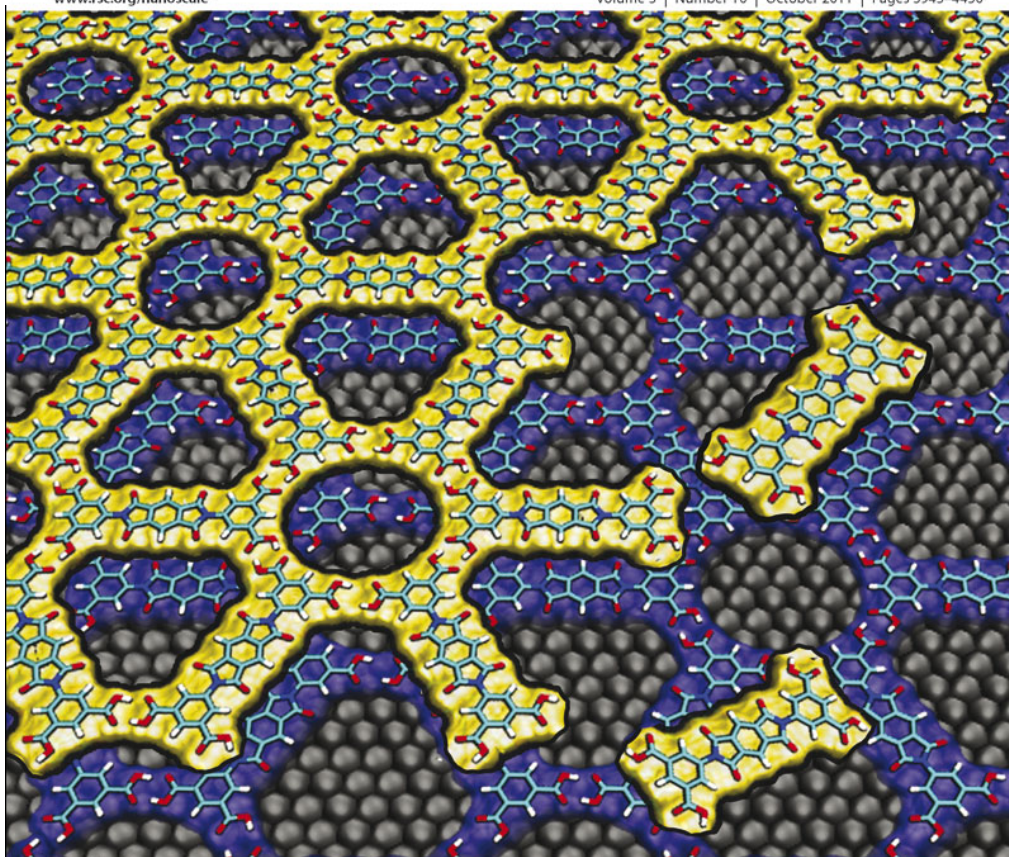
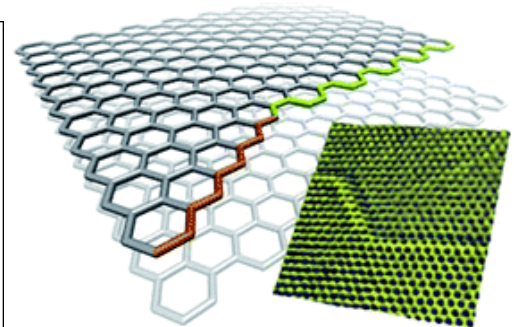




# Nanoscale

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**COVER ARTICLE**  
Cecchini, Samori *et al.*  
Self-templating 2D supramolecular  
networks: a new avenue to reach  
control over a bilayer formation



2040-3364 (2011) 3:10;1-R



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| 1            |  | Metais alcalino-terrosos |  | Semi-metais            |  | Hg Líquido         |  |                 |  | 2               |  |
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| 3            |  | 4                        |  | Metais de transição    |  | Rf Desconhecido    |  |                 |  | 10              |  |
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| Na Sódio     |  | Mg Magnésio              |  |                        |  |                    |  |                 |  | Ar Argônio      |  |
| 19           |  | 20                       |  | 3B                     |  | 4B                 |  | 5A              |  | 6A              |  |
| K Potássio   |  | Ca Cálcio                |  | 21 Sc Escândio         |  | 22 Ti Titânio      |  | 7 N Nitrogênio  |  | 8 O Oxigênio    |  |
| 37           |  | 38                       |  | 23 V Vanádio           |  | 24 Cr Crômio       |  | 15 P Fósforo    |  | 9 F Flúor       |  |
| Rb Rubídio   |  | Sr Estrôncio             |  | 41 Nb Nióbio           |  | 42 Mo Molibdênio   |  | 14 C Carbono    |  | 17 Cl Cloro     |  |
| 55           |  | 56                       |  | 43 Tc Tecnécio         |  | 44 Ru Rutênio      |  | 33 As Arsênio   |  | 10 Ne Neônio    |  |
| Cs Césio     |  | Ba Bário                 |  | 75 Re Rênio            |  | 76 Os Ósmio        |  | 34 Se Selênio   |  | 18 Ar Argônio   |  |
| 87           |  | 88                       |  | 79 Au Ouro             |  | 80 Hg Mercúrio     |  | 35 Br Bromo     |  | 36 Kr Criptônio |  |
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|              |  |                          |  | 391 Uus Ununséptio     |  | 39                 |  |                 |  |                 |  |

carbono

|    |    |    |
|----|----|----|
| 6  | C  | 6  |
| 14 | Si | 14 |
| 32 | Ge | 32 |

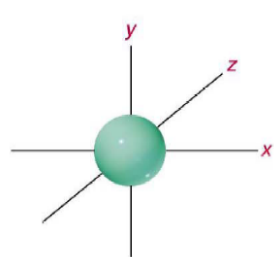
www.tabelaperiodicacompleta.com



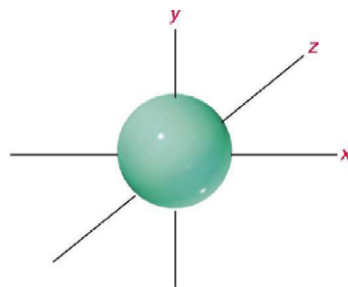


# CARBONO $1s^2 2s^2 2p^2$

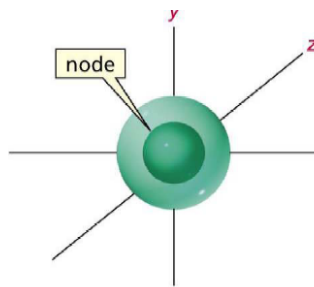
- Grande número de compostos
- Diferentes tipos hibridização
- Não-metálicos & não-magnéticos



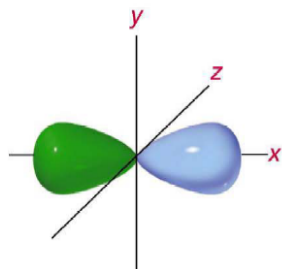
1s atomic orbital



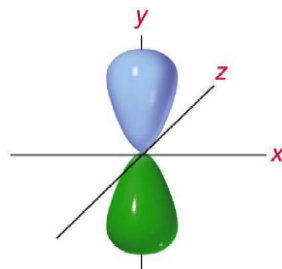
2s atomic orbital  
node not shown



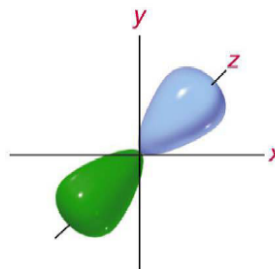
2s atomic orbital  
node shown



$2p_x$  orbital

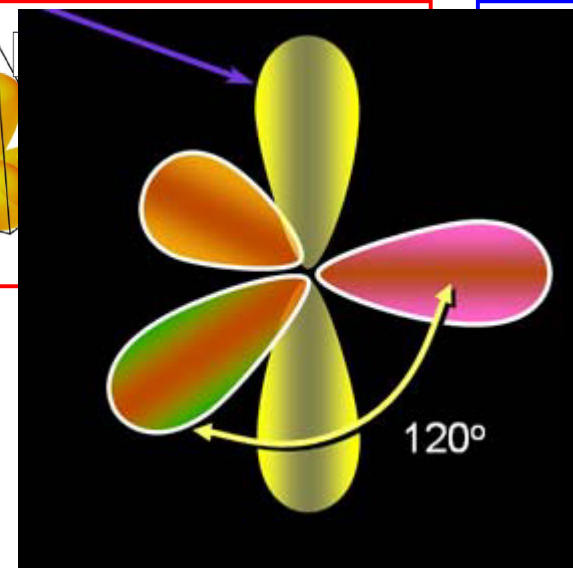
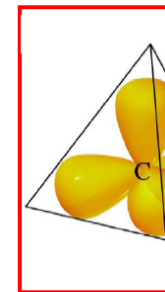


$2p_y$  orbital

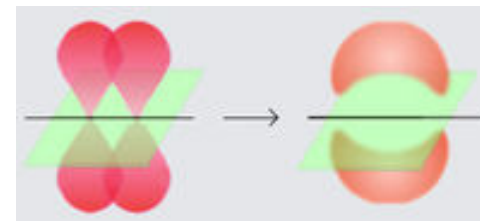


$2p_z$  orbital

## Orbitais híbridos



[movie](#)

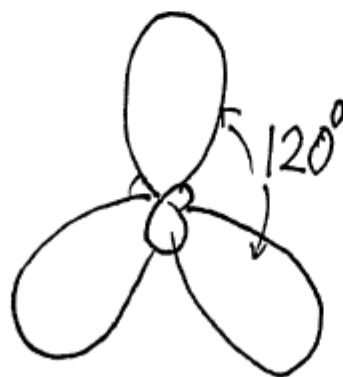
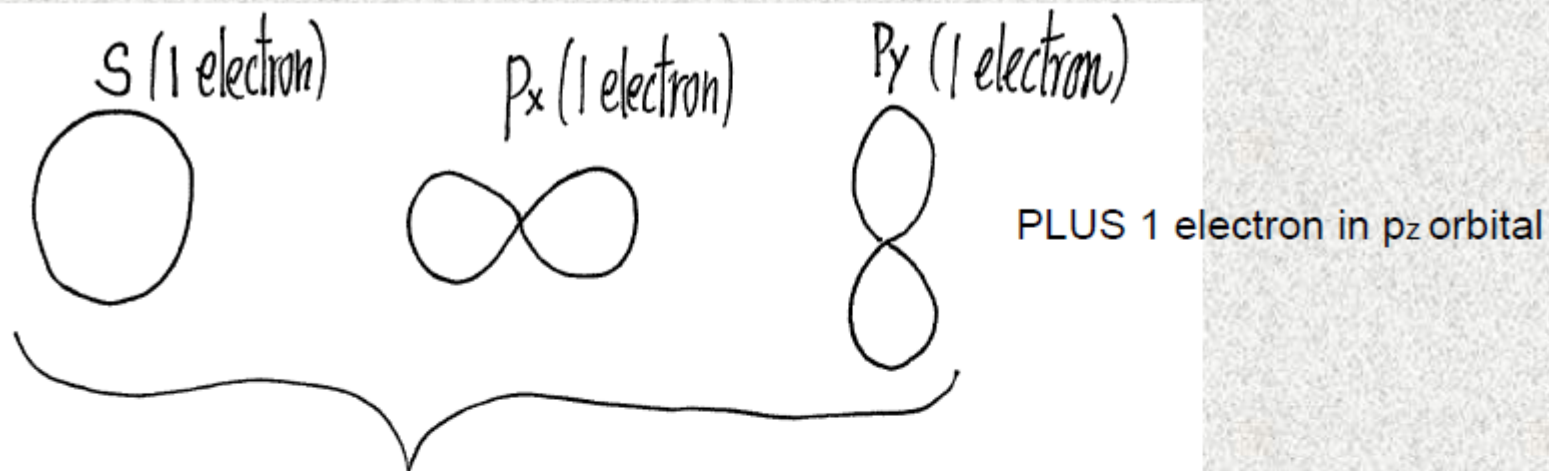


$\pi$ -bond





In Graphene, it is two-dimensional.



There is 1 electron in each of the 3 hybridized  $sp^2$  orbitals.

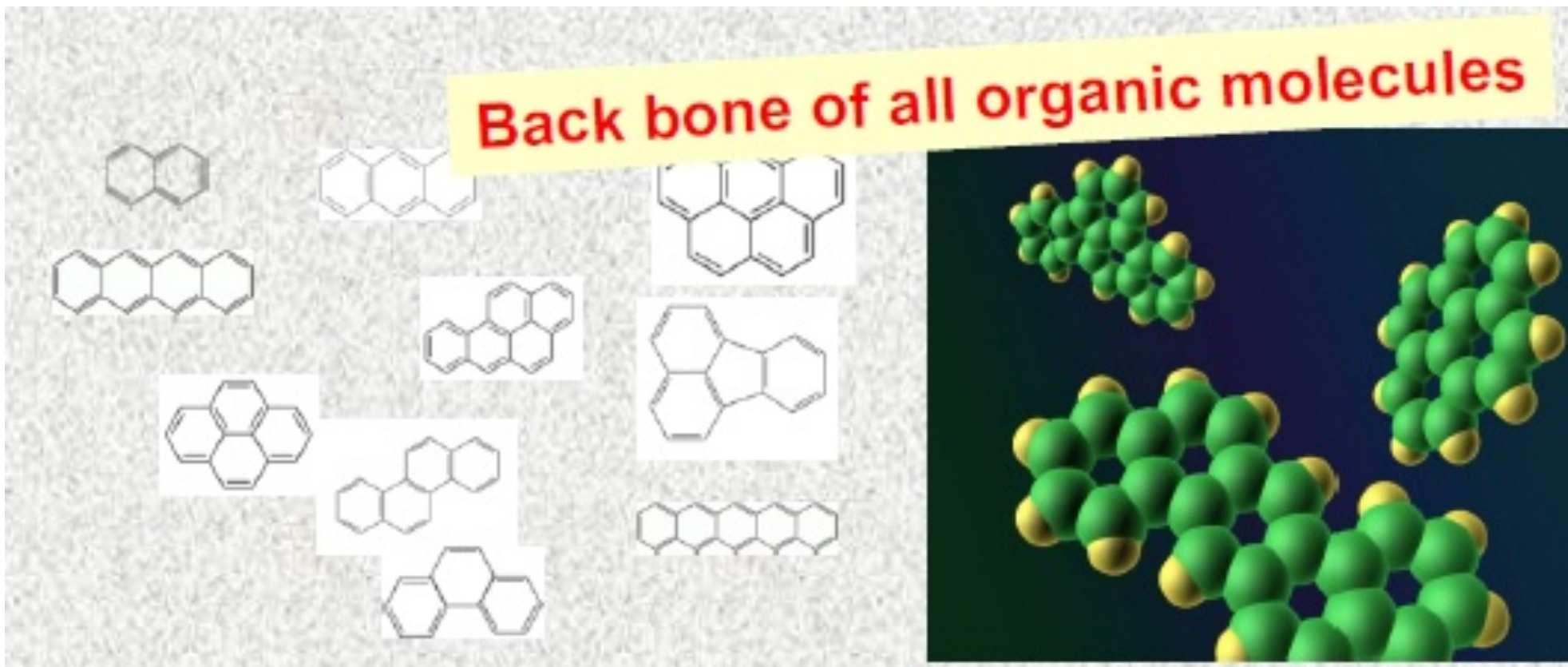
**Strong covalent bonds** are formed when neighboring atoms come close.

Highly dimensional  $\Rightarrow$  expected to form honeycomb lattice

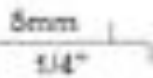


# CARBONO

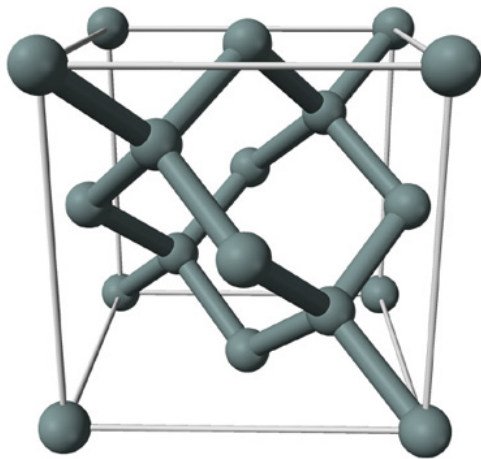
**Back bone of all organic molecules**



# Diamante

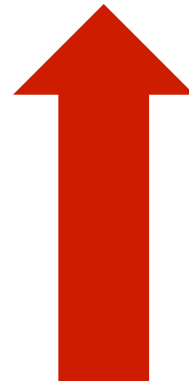
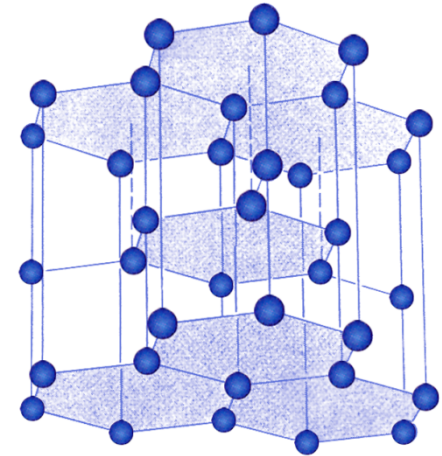


- Hibridização  $sp^3$
- Isolante
- Transparente



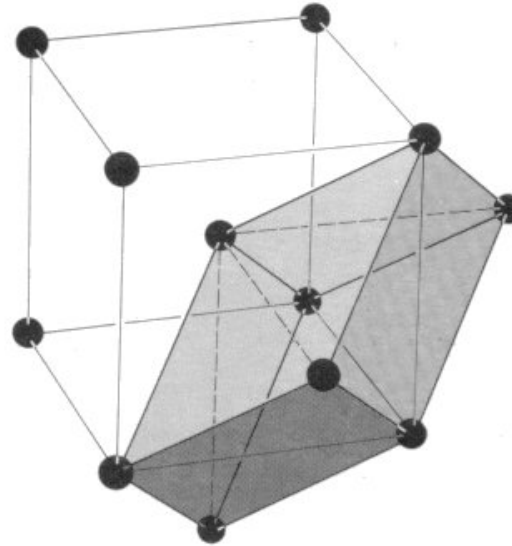
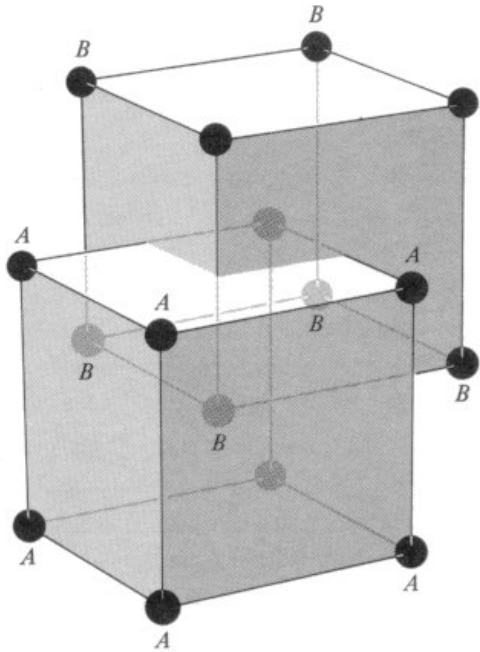
# Grafite

- Hibridização  $sp^2$
- Semimetal





## Átomos – Moléculas - Cristais



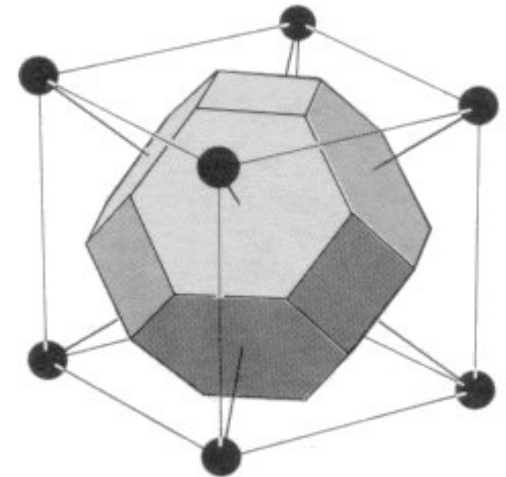
**Simetrias**

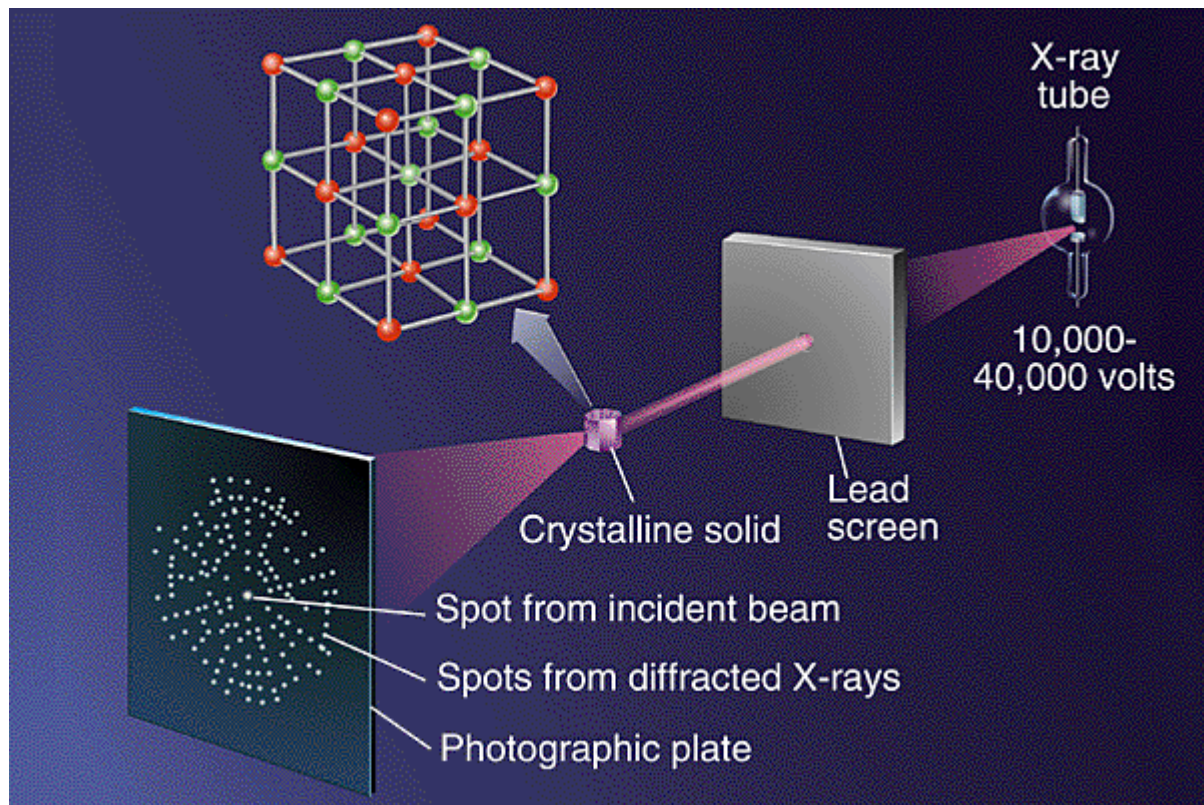
**Redes Diretas**

**Redes Recíprocas**

**Redes Cristalinas: Teorema de Bloch – simplificações matemáticas -**

**\* Resolver o problemas de autovalores de energia**



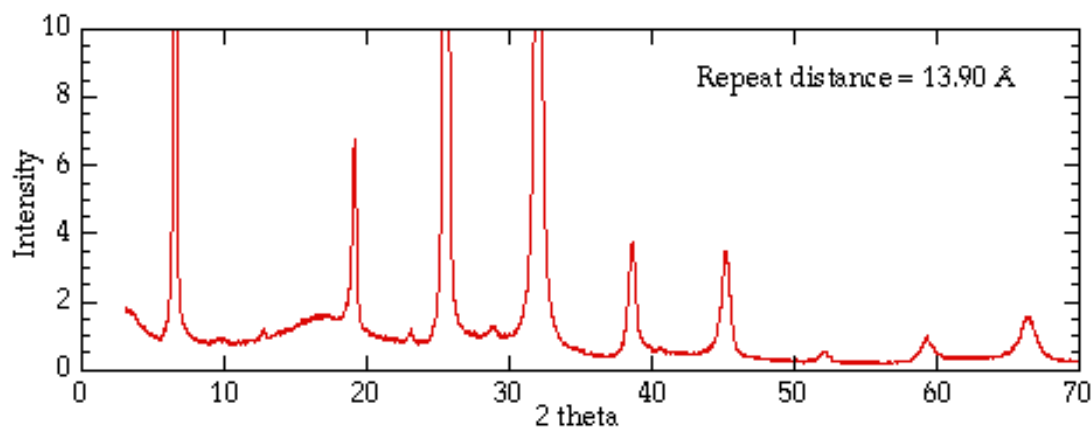


**Descobrimos a estrutura do sistema cristalino**

**MEDIDAS DE RAIO-X**

**REDES CÚBICAS**

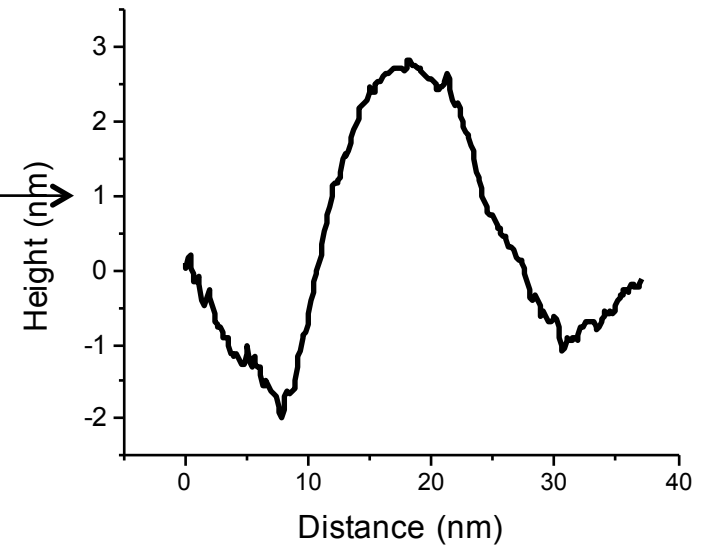
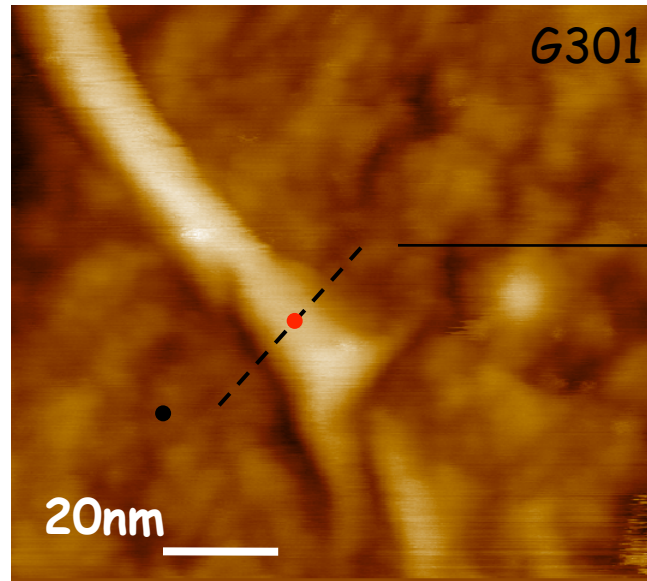
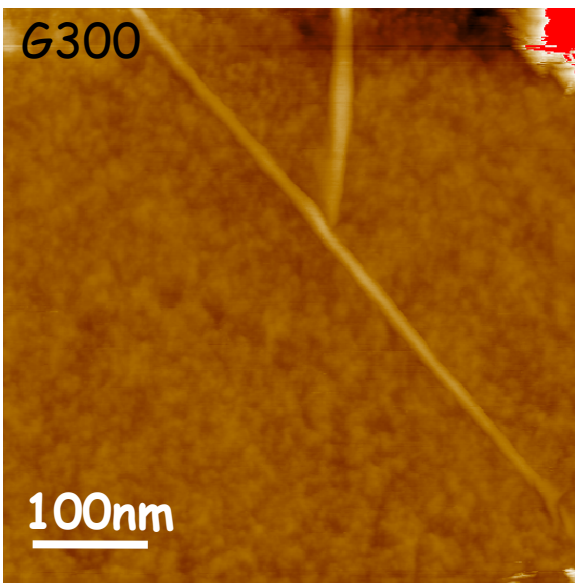
**REDES HEXAGONAIS**



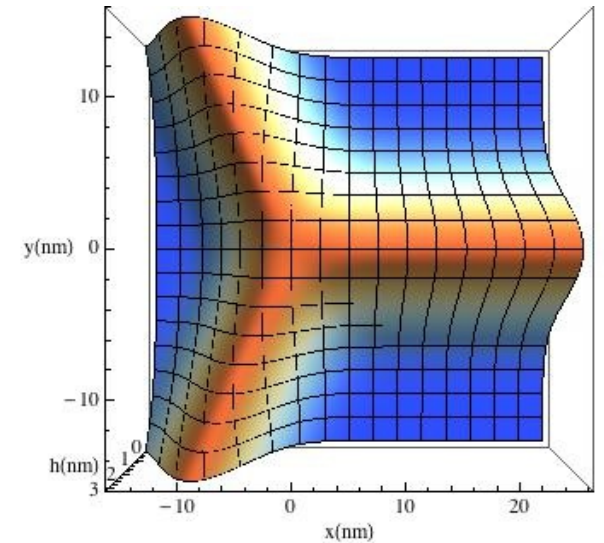
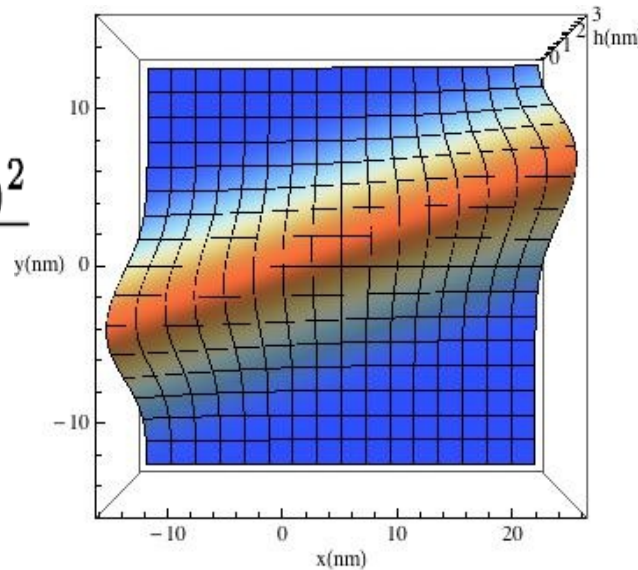
**ANÁLISES ESPECTRAIS**



# Ripples seen by STM



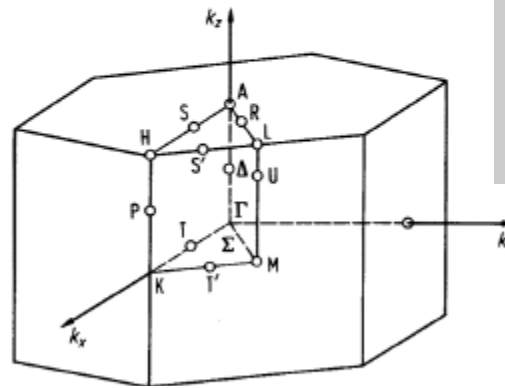
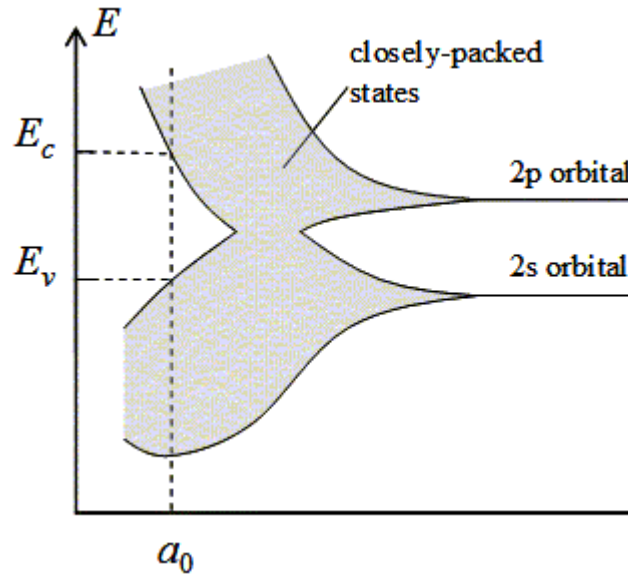
$$h[\phi] = Ae^{\frac{-(x(-\sin[\phi]) + y\cos[\phi])^2}{b^2}}$$





# BANDAS DE ENERGIA

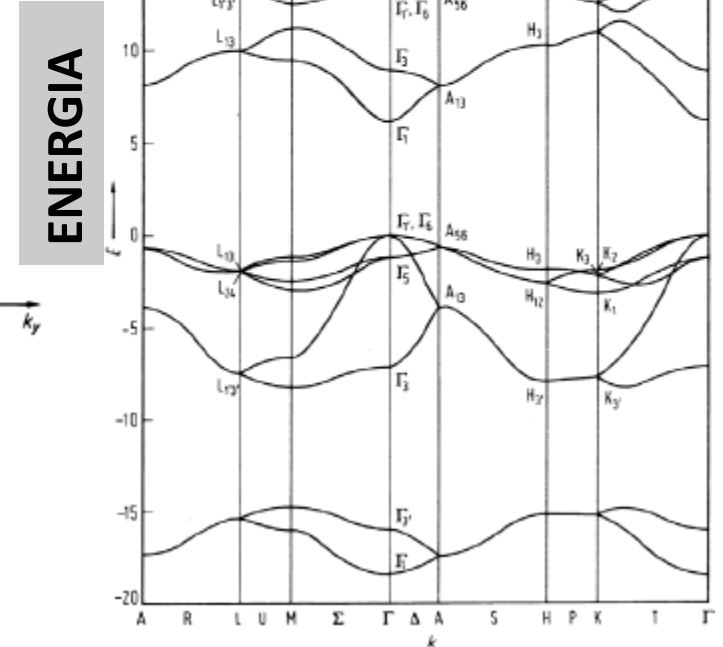
APh 114b Lecture 4  
Solid State Physics



$$H\psi = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) \right] \psi = E\psi$$

## Gaps de energia - SEMICONDUTOR

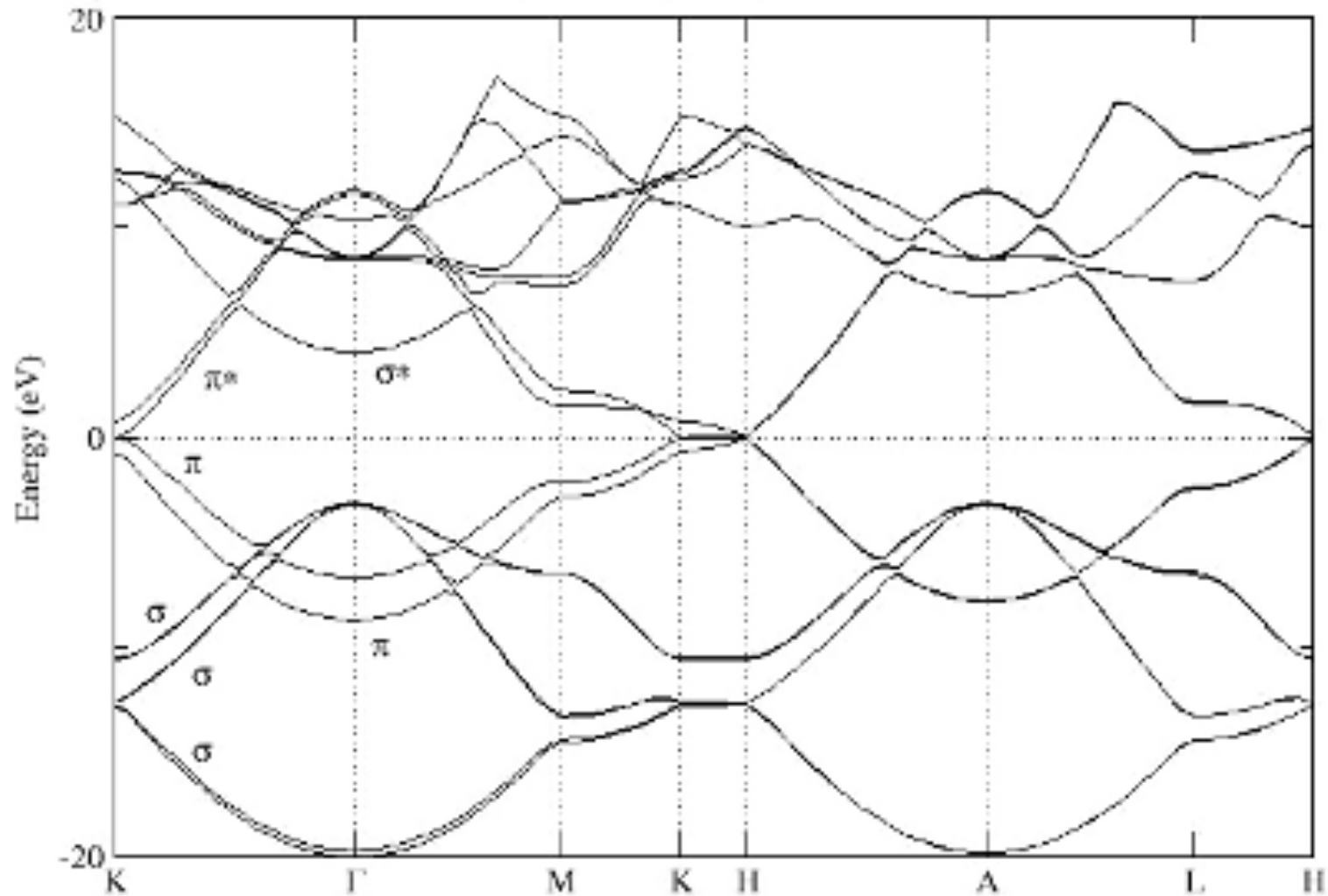
Band structure of AlN (Wurtzite) at 300 K



VETOR DE ONDA K

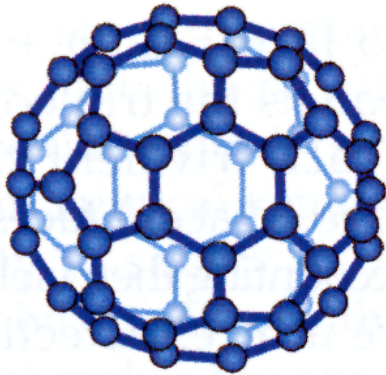


# ESTRUTURA DE BANDA DO GRAFITE - DFT

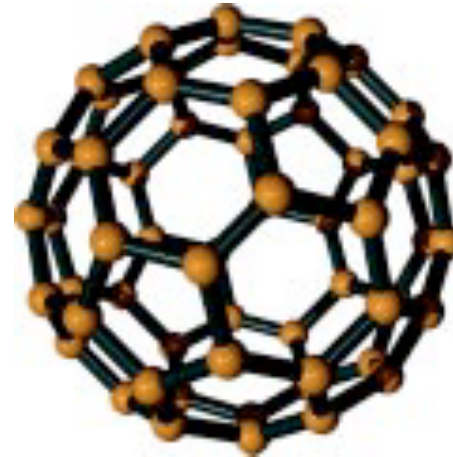
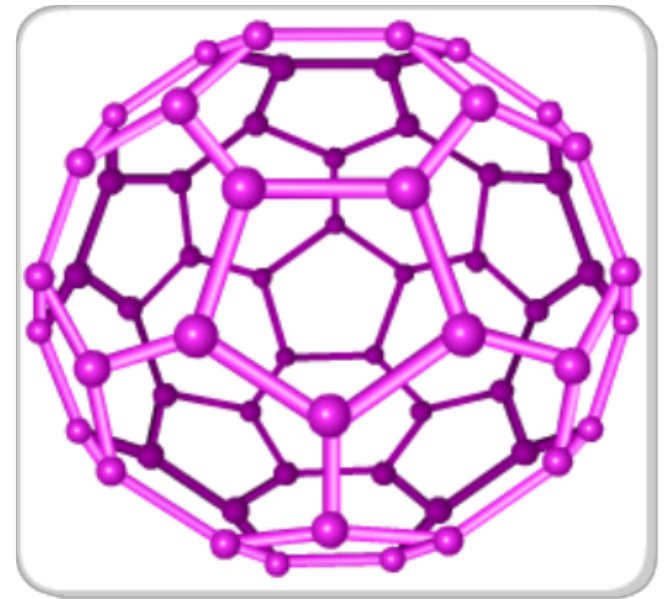


(1950) necessidade da indústria espacial e de naves: fibras mais forte, resistentes e mais leves para serem usadas nos materiais de construção com propriedades mecânicas superiores

## Novas formas de Carbono



Fullerenes “Buckyballs”  
 $C_{60}$   $sp^2$  hybridization



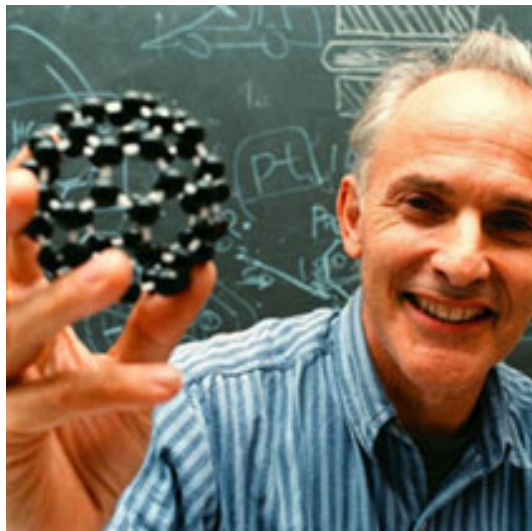
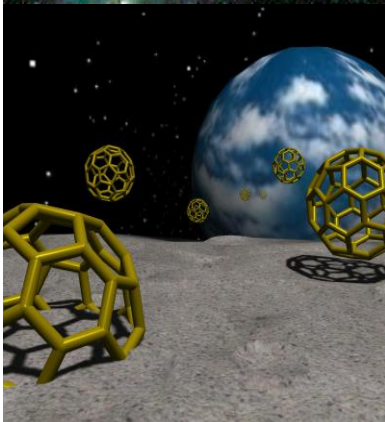
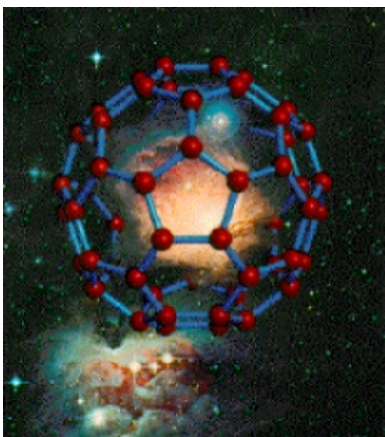
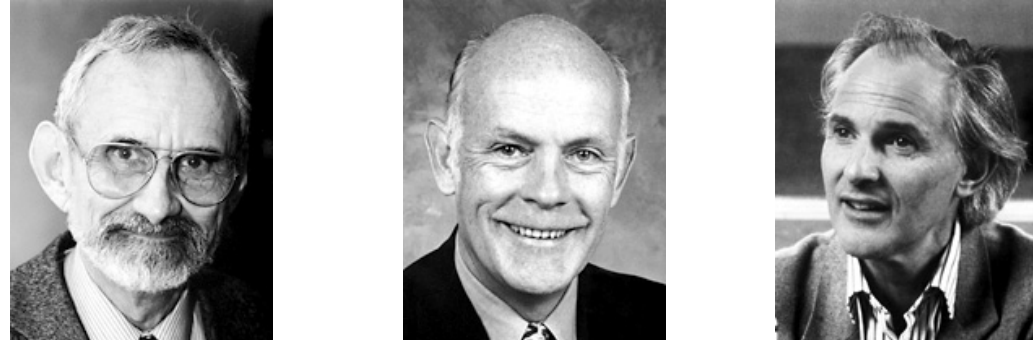


MUSEU DA  
CIÊNCIA EM  
LISBOA





## 1996 - Nobel Price Chemistry



Rice University, USA 1984  
Curl  
O'Brien, Smalley, Kroto and Heath



# Aplicações

A molécula de  $C_{60}$  pode ligar um grande número de átomos de Hidrogênio (até 1 H para cada C) sem romper a estrutura. Esta propriedade sugere que **uckyballs** possam ser um meio eficiente de armazenar H, mais acessível a economia geral.

2005 – REPORT de revisão - propôs que formas modificadas de buckminsterfullerene chamadas de **organometallic uckyballs (OBBs)** podiam ser usadas como veículos de “armazenador de H de alta densidade e temperatura ambiente”.

No **meio médico**, elementos como o hélio (que pode ser detectado em quantidades minutas) podem ser usados como uckyballs impregnados de traçadores químicos. Buckminsterfullerene podem também **inibir o vírus HIV**. Em particular,  $C_{60}$  inibe uma enzima chave na imunodeficiência humana, que o vírus conhecido como HIV-1 protease; isto pode inibir a reprodução do vírus de HIV em células imunes.

As propriedades ópticas de absorção do  $C_{60}$  se encaixam no espectro solar que favorece os filmes baseados em  $C_{60}$  para aplicações fotovoltaicas. Conversões de eficiências até 5.7% tem sido reportadas em células de polímeros de  $C_{60}$

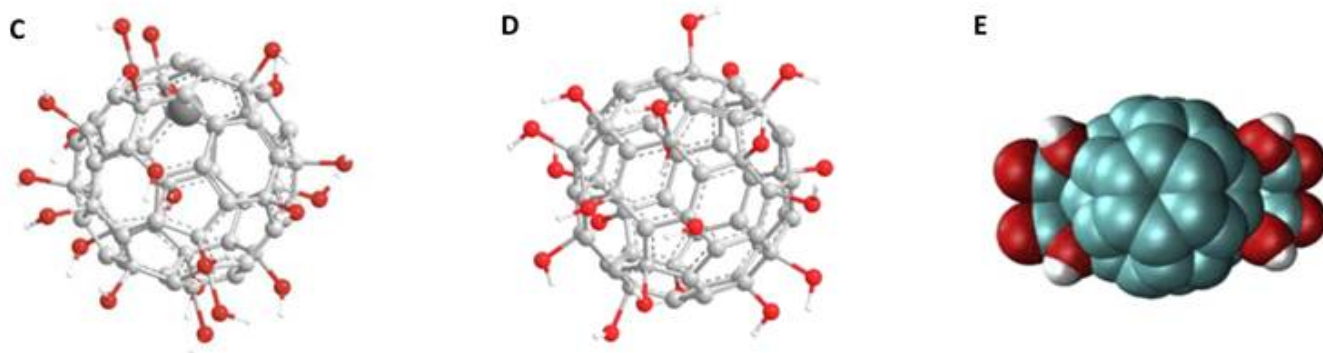
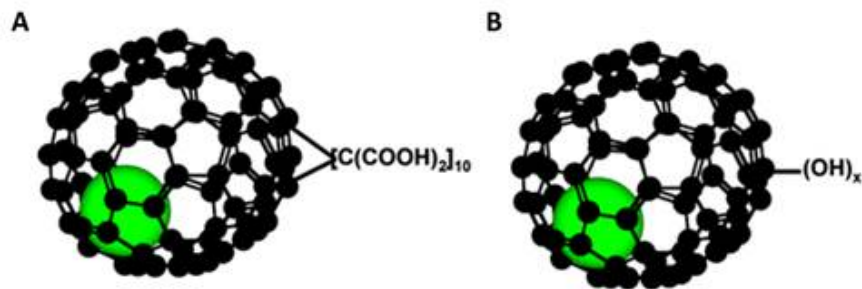
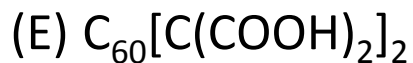
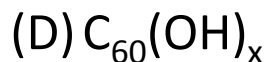


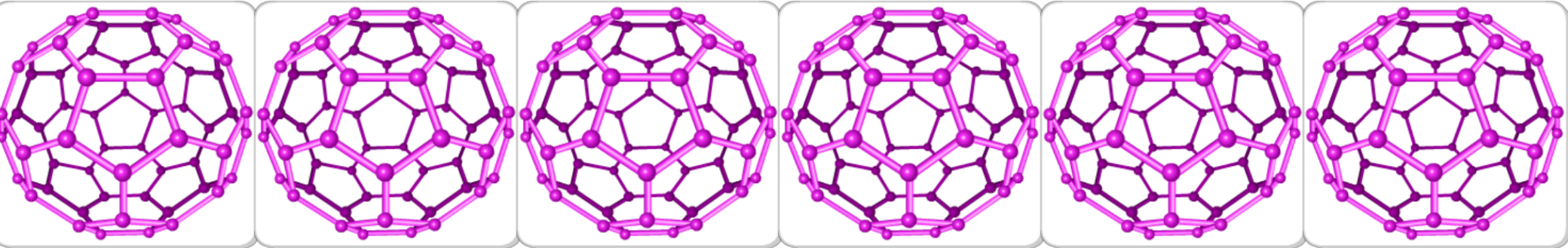


**Theranostics 2012; 2(3):238-250. Review**  
**Applications of Functionalized Fullerenes in Tumor Theranostics**  
**Zhiyun Chen, Lijing Ma, Ying Liu, Chunying Chen**

**Magnetic resonance imaging**

MRI is a versatile, non-invasive medical diagnostic technique that can provide both physiological and anatomical information, while not requiring the use of ionizing radiation. In addition, in many applications it is often the most sensitive method available to depict soft tissues. Therefore, it has been extensively used for brain and central nervous system imaging, for assessing cardiac function and for detecting abnormal tissues such as tumors

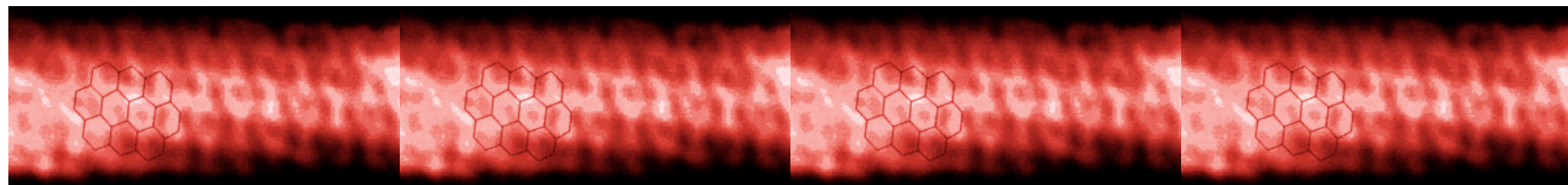


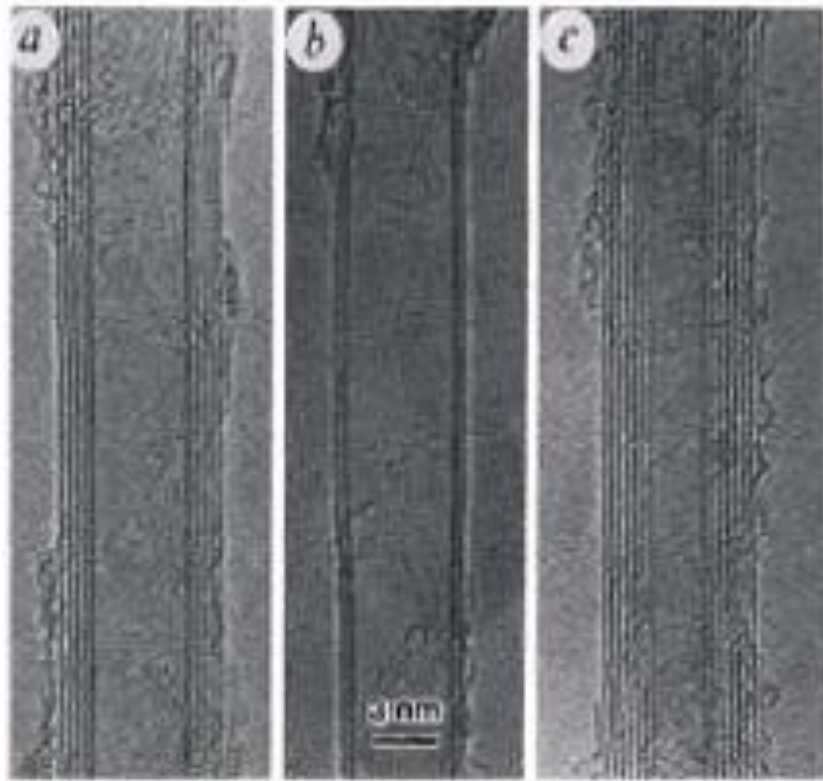


DO FULERENO

AO

NANOTUBO DE CARBONO





Fibras de Carbono

M. Endo, 1976

**Nanotubo de Paredes múltiplas  
MWNT**

**S. Iijima, Nature 354, 56 (1991)**



The first TEM evidence for the tubular nature of some **nano-sized carbon filaments** is believed to have appeared **in 1952** in the Jour. of Phys. Chem. **of Russia**, which may explain why the related papers are not well known and cited. Due to the cold war, access to Russian scientific publications for Western scientists was not easy at that time, and the use of the Russian language was pretty discouraging anyway!

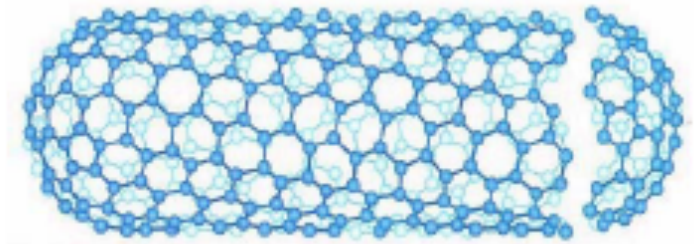






**Possibilidade de  
formar estruturas  
tubulares de Carbono**

**CN propriedades de simetria e  
modelo 1991 DRESSELHAUS**

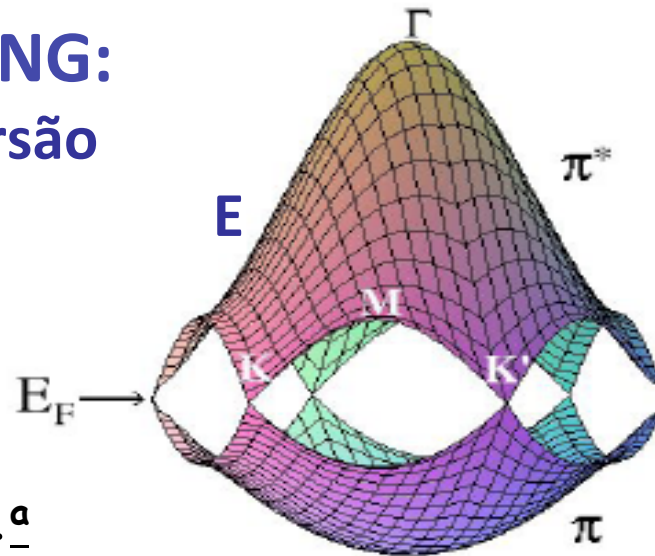
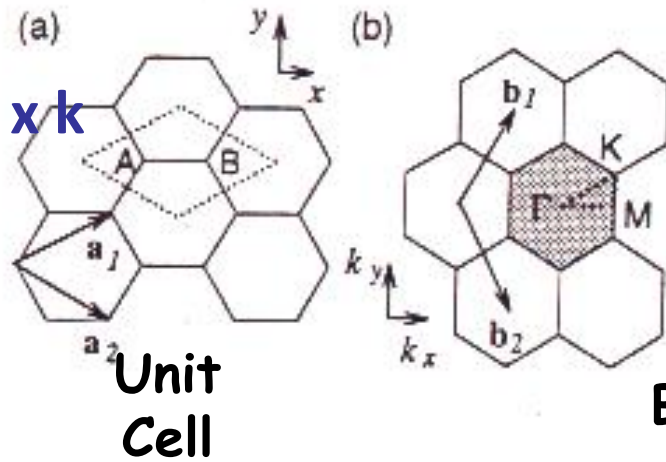


**Nanotubos de Carbono, 1991**

**1991 ➡ S. Iijima (NEC Fund. Research Lab)  
1976 Endo – publicações de resultados de CNs**



# •MODELO TIGHT-BINDING: cálculo da relação de dispersão



$\det[H-ES]=0$  secular equation

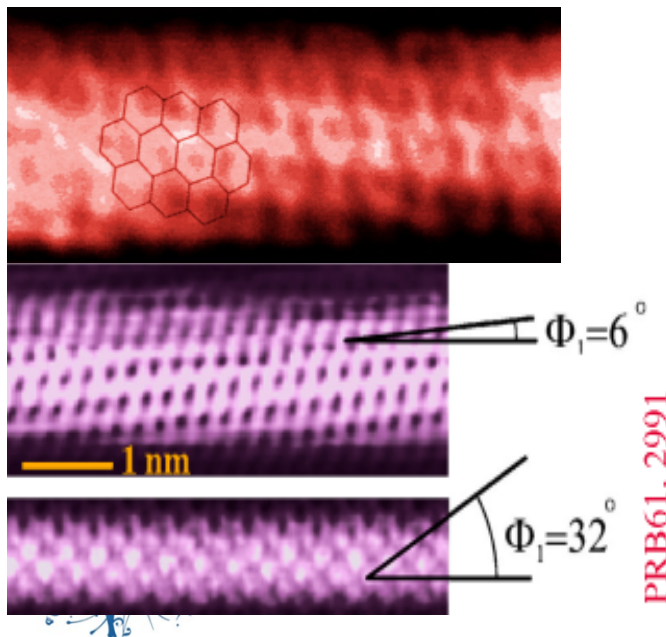
## Nanotubes

$$C \cdot k = 2\pi q$$

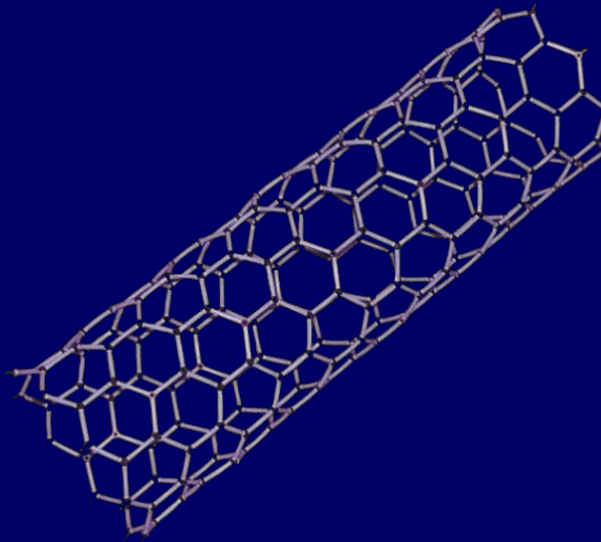
M. S. Dresselhaus et al, PRB 46, 1804 (1992)

## • Condições de contorno periódicas

- Armchair (n,n)  $K_{xq} = 2\pi/a\sqrt{3} q/n$  ( $q = 1, \dots, 2n$ )
- Zigzag (n,0)  $K_{yq} = 2\pi/a q/n$  ( $q = 1, \dots, 2n$ )

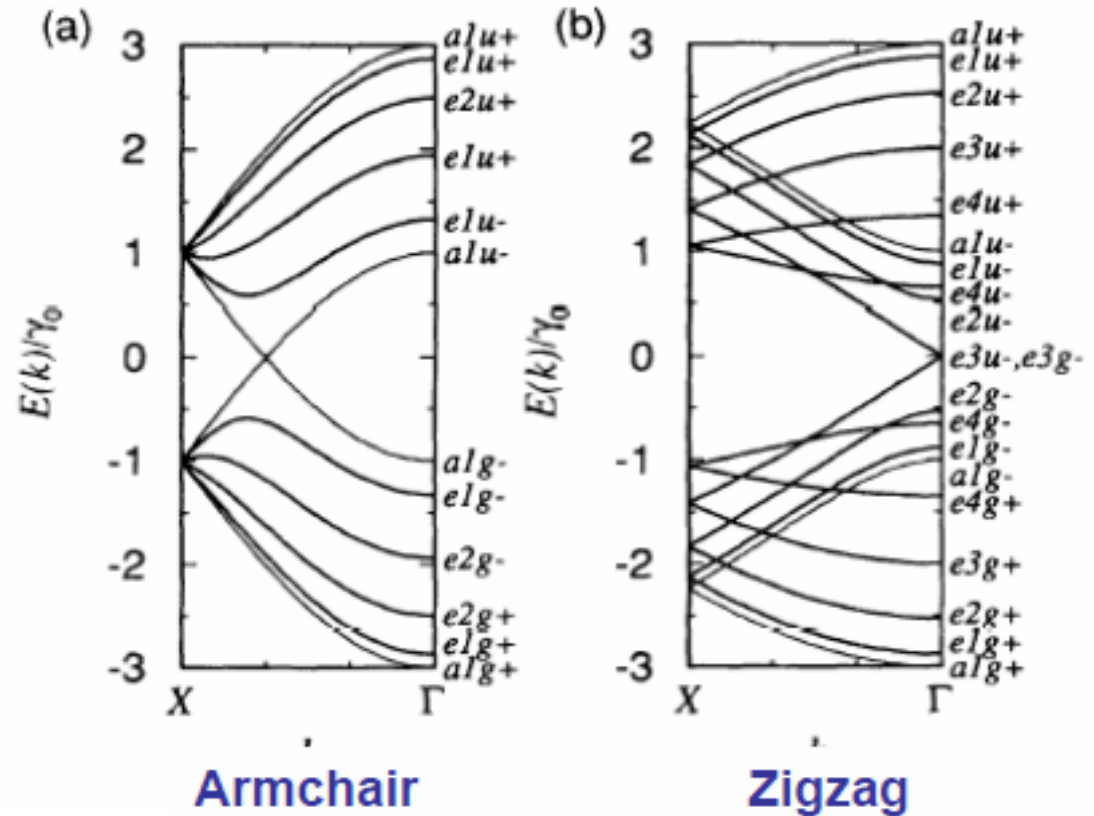
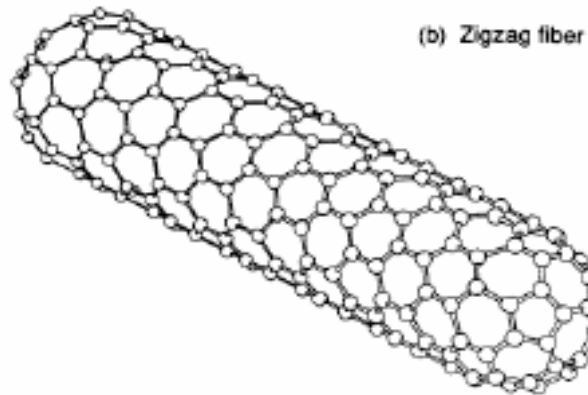
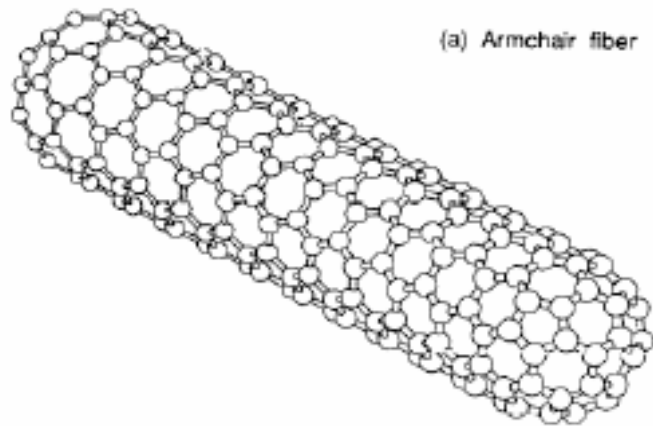


# Band Structure of Carbon Nanotubes





## Band structure of Carbon Nanotubes at 300 K

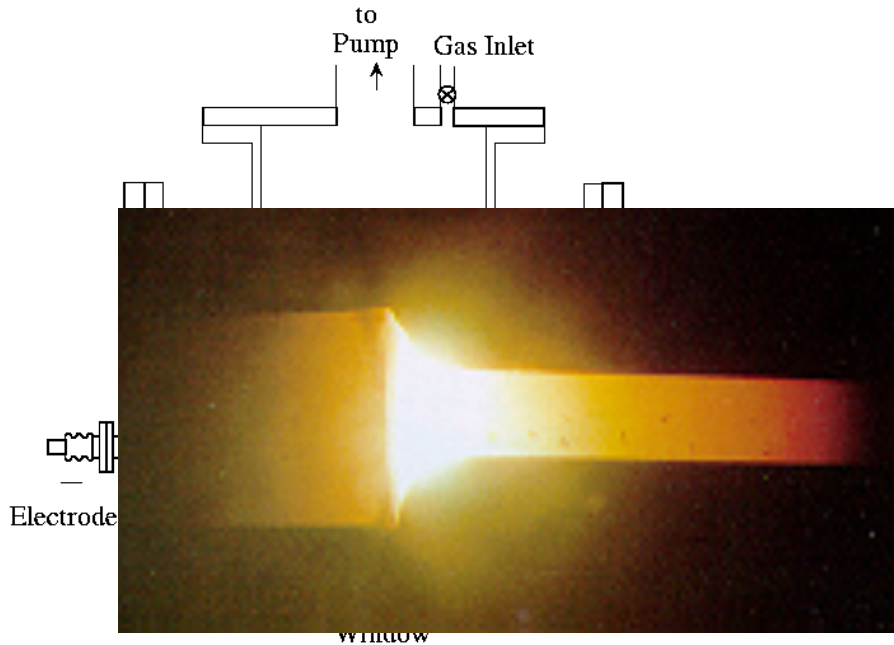


# Processos de Síntese

- Usado por S. Iijima in 1991

## DESCARGA DE ARCO

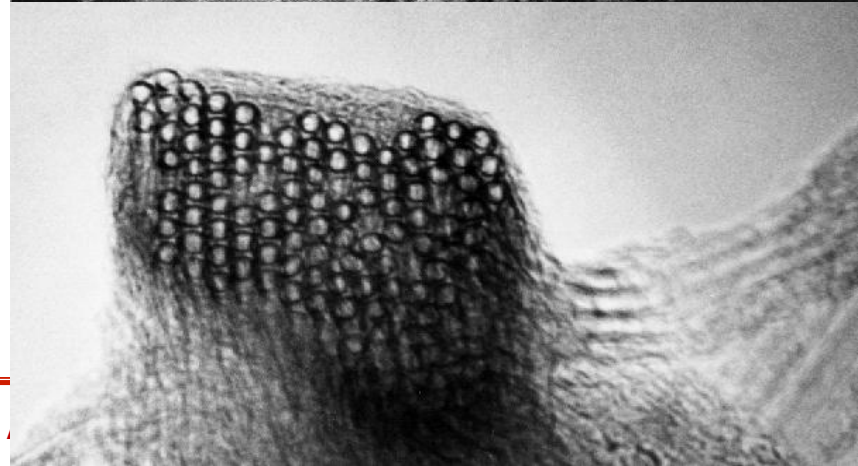
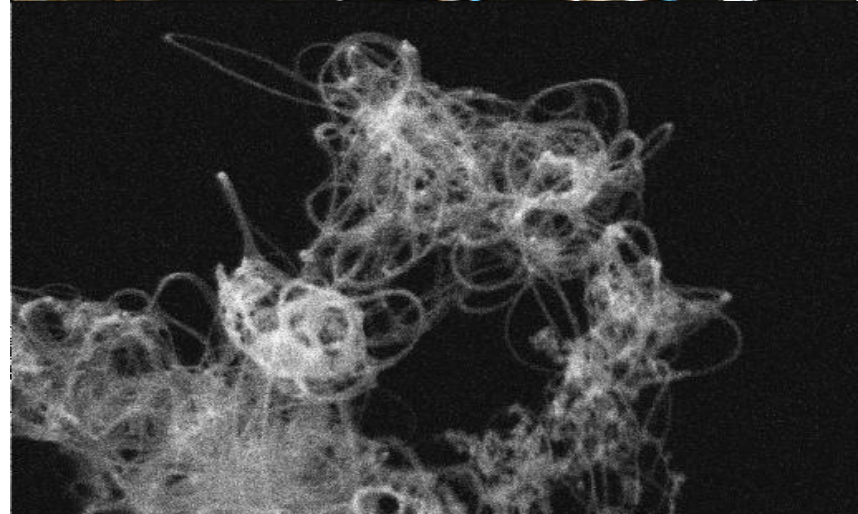
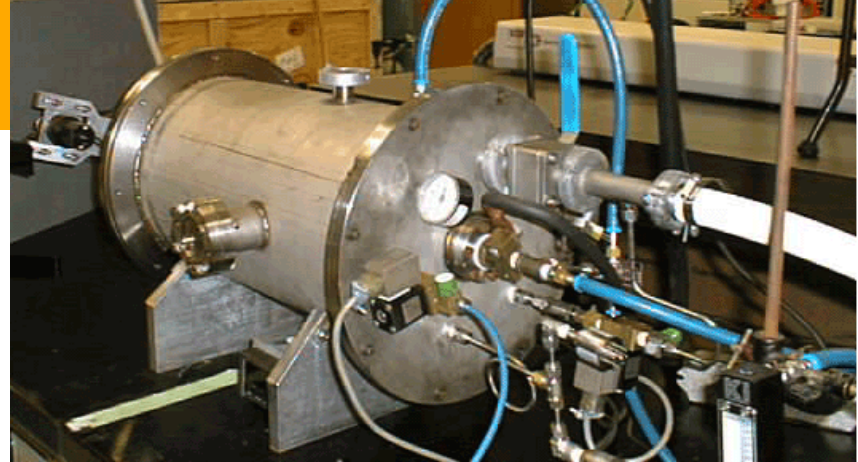
$T=1000^{\circ}\text{C}$

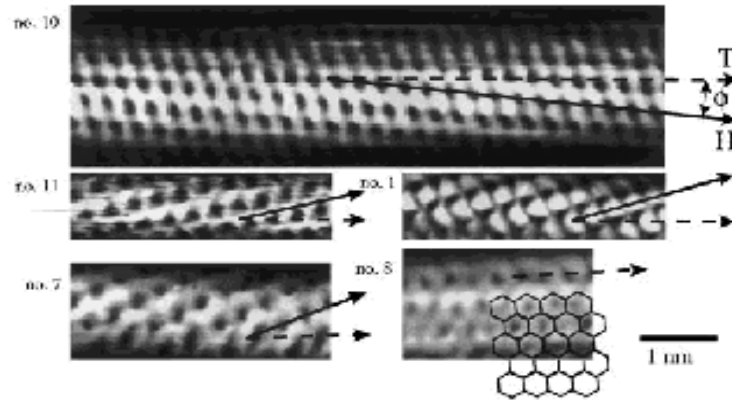
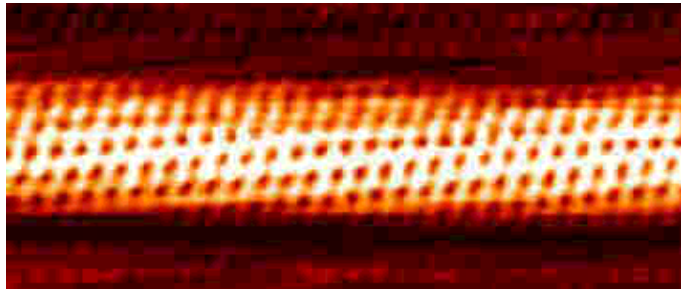
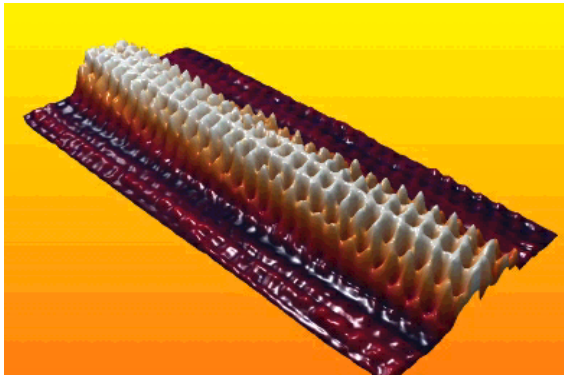


Y. Saito *et al.*  
*Phys. Rev.* 48 1907 (1993)



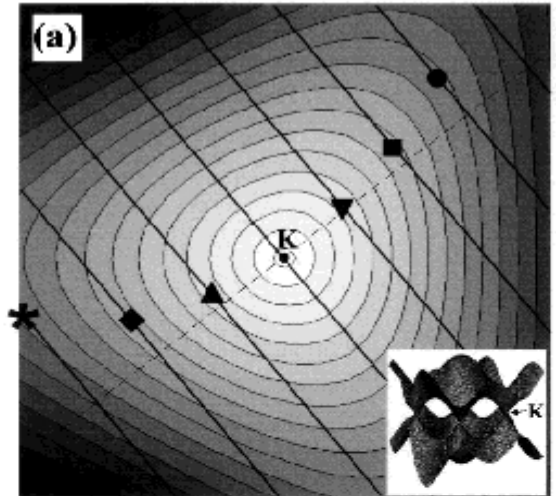
Smalley *et al.* (1996)



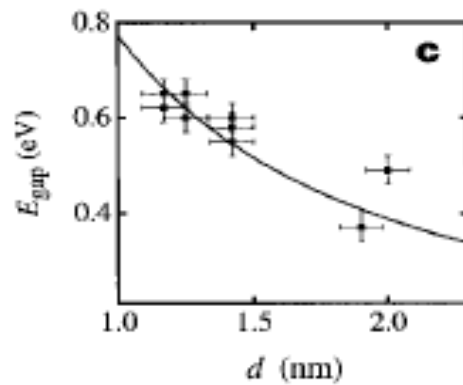
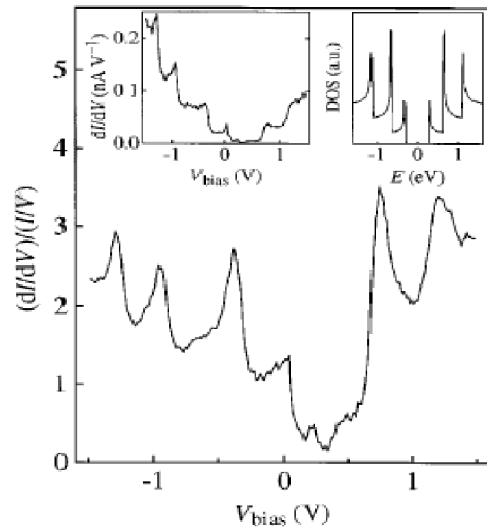


# STM/STS caracterização

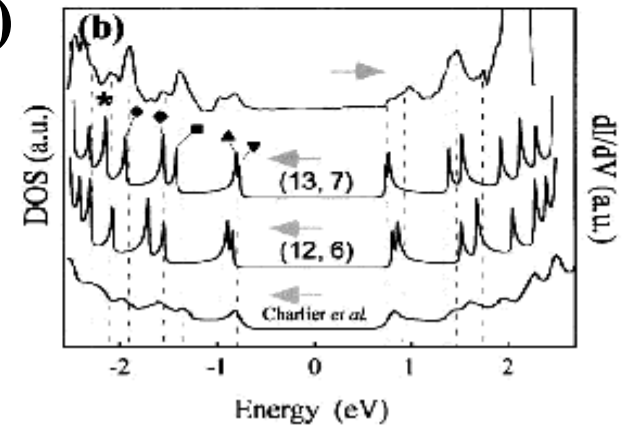
P. Kim et al.,  
PRL 82, 1225 (1999)



cutting  
lines  
(13,7)

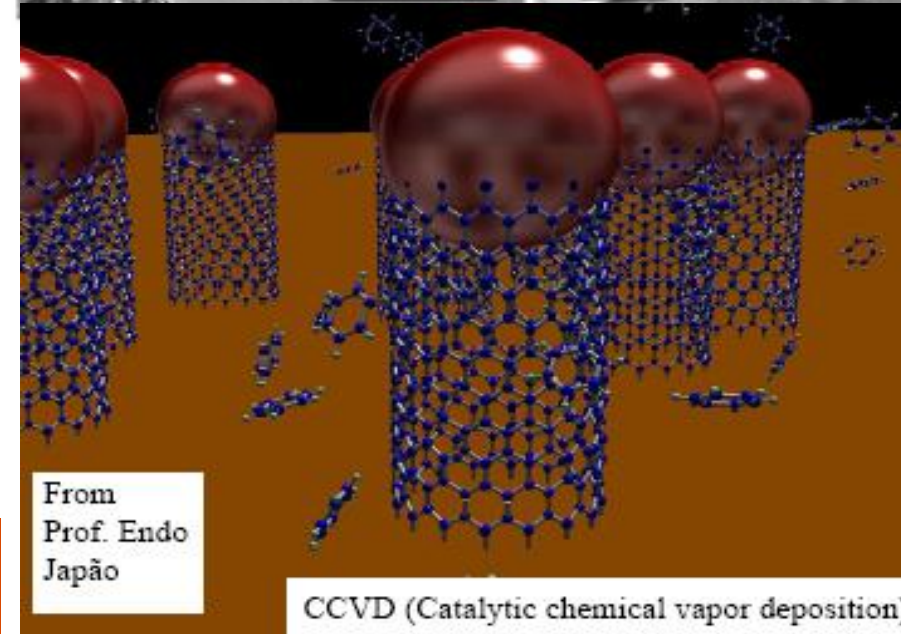
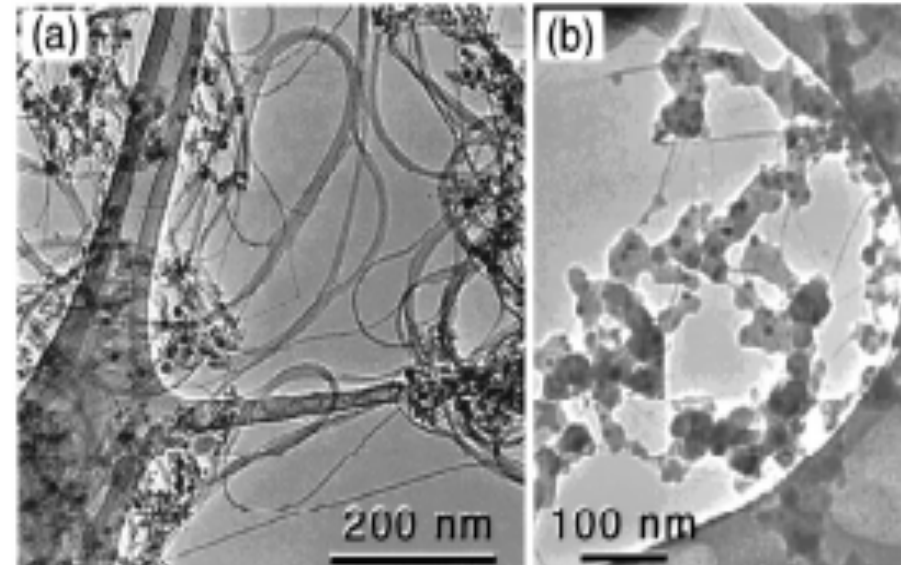
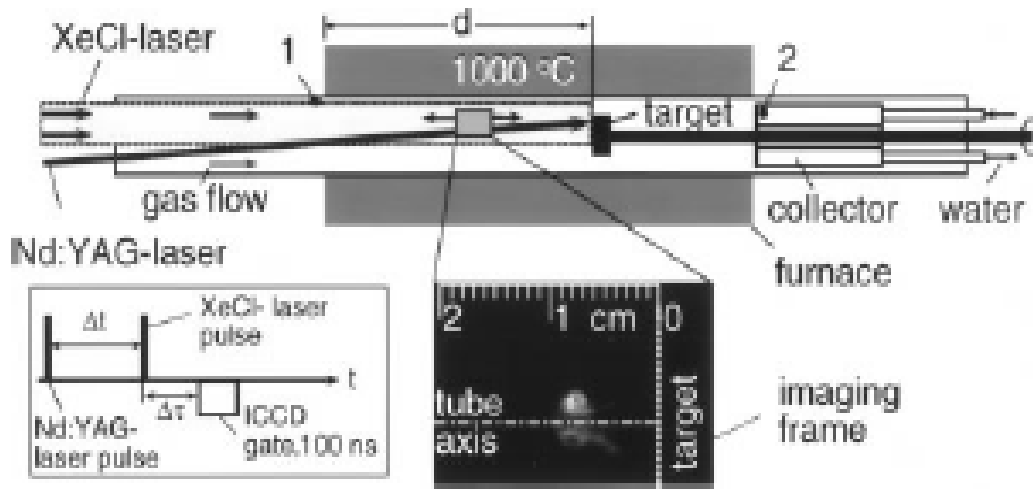


J. W. G. Wildoer et al., Nature 391,  
59 (1998)





# Evaporação a Laser ➡ tubos de parede única - SWCN



Além dos CNs:

C amorfos, grafite,  
catalíticos, etc

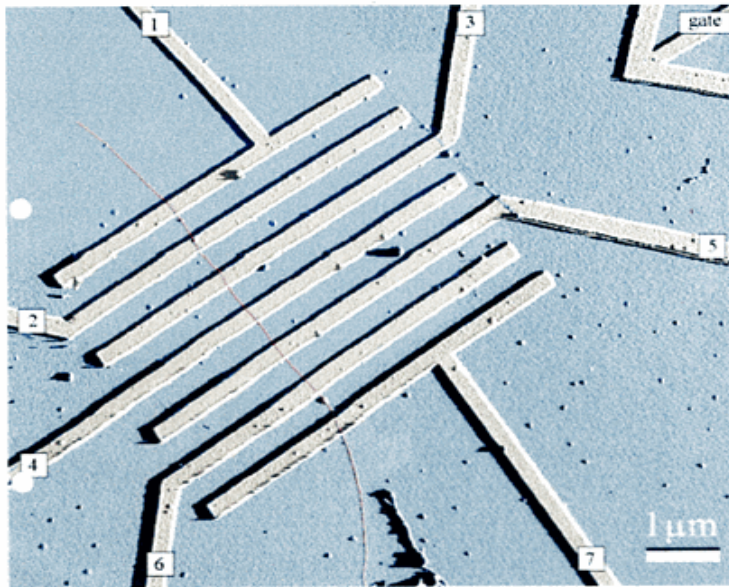
**CVD**



# Nanoeletrônica... Transistores à temperatura ambiente

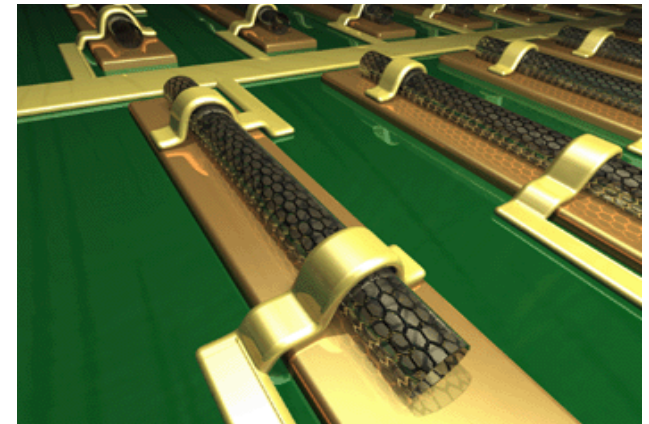
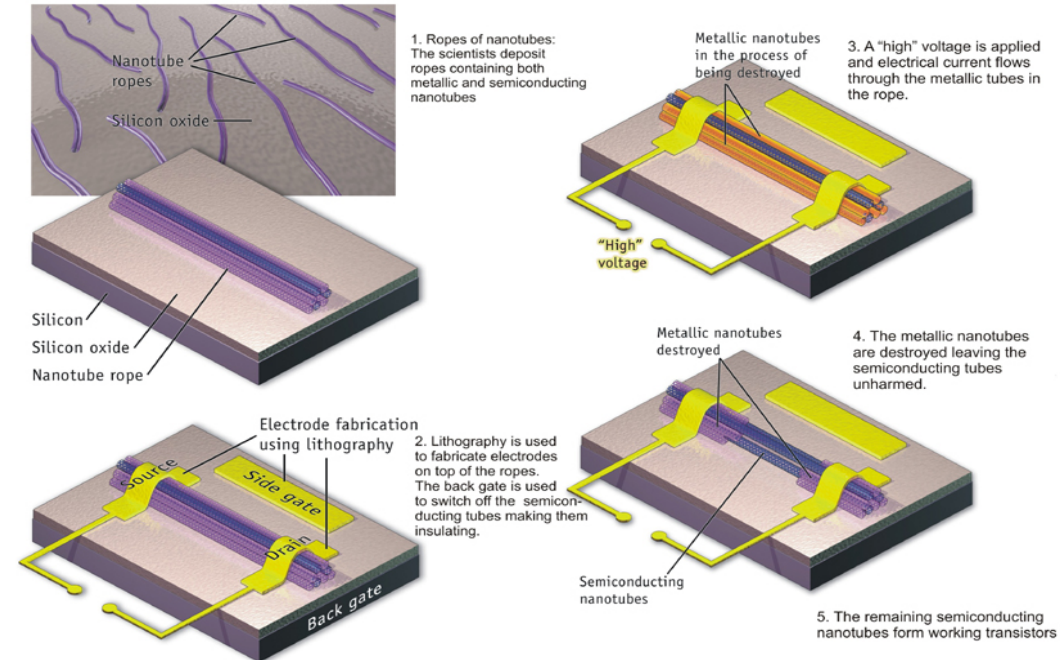
## Multiprobe measurements on a single nanotube

### An individual carbon nanotube on 7 electrodes:



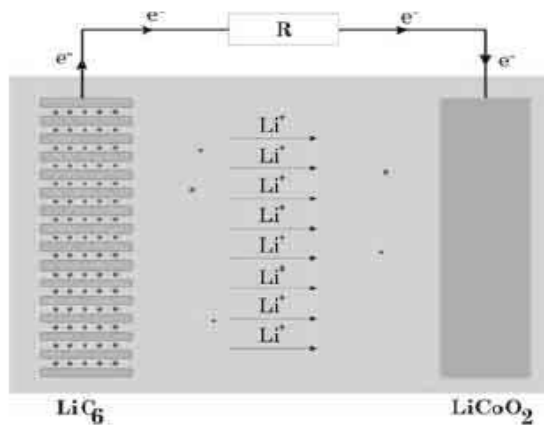
This allows 2-probe and 4 probe experiments on a single nanotube molecule

DELFT Group  
Bezryadin *et al.* PRL 1998  
Viewgraph courtesy of  
Cees Dekker

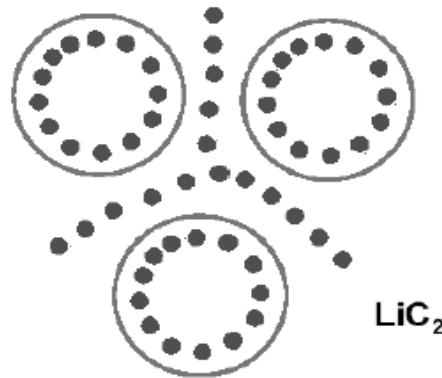




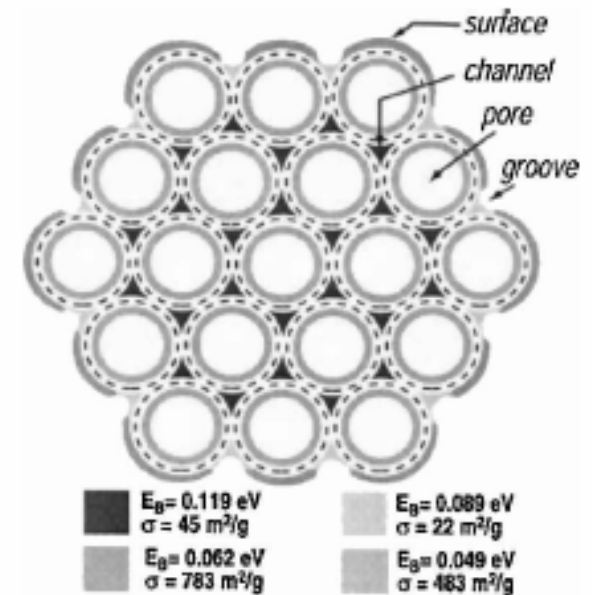
# Baterias de LITTIUM



Lithium "rockingchair" battery



LiC2 Nanotube-based anode



Aumento Significativo da vida média

Y. Ando, I. Ijiima, NEC, J,

- até 3 x a capacidade de armazenamento

-



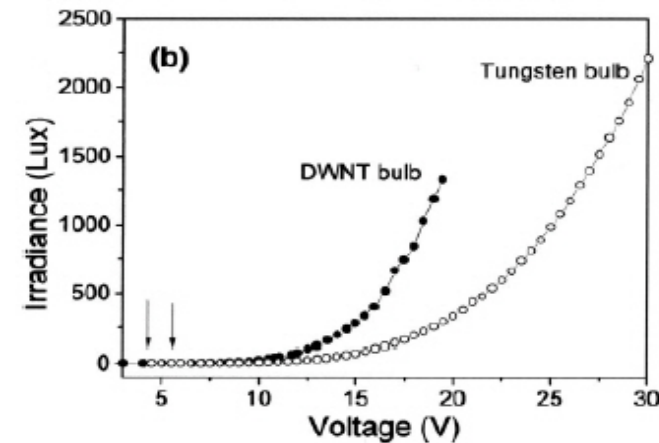


# Propriedades Ópticas de CNTs

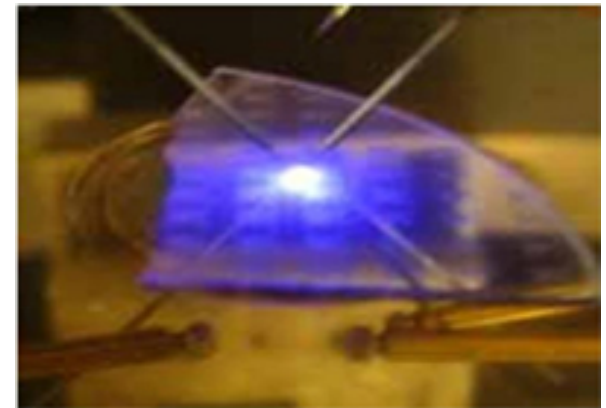
- ❖ STM/AFM microscópios
- ❖ Sensores de gás
- ❖ Armazenadores de H
- ❖ Dispositivos Nanoeletrônicos
- ❖ Emissores de campo
- ❖ Dispositivos Fotônicos

Conhecimento das propriedades ópticas e absorção e emissão

Monitores Coloridos de CN  
(Samsung, Choi et. al.)



LED made of CN filament



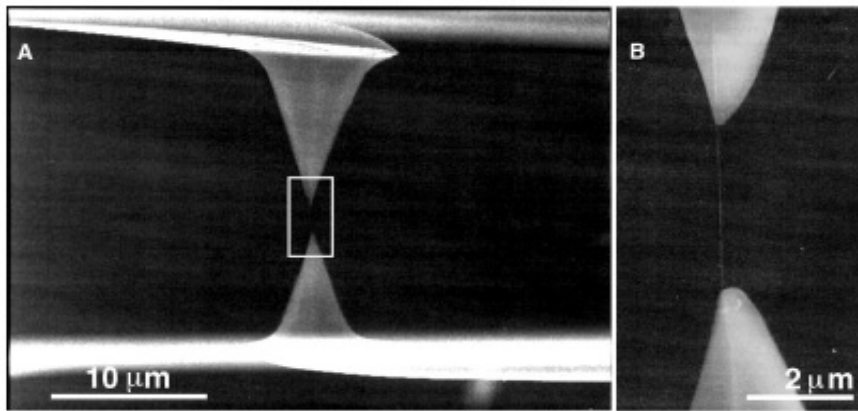
# Propriedades Mecânicas

Leves, rígidos e flexíveis, reconstrução....

SWCN - Densidade  $1,4 \text{ g/cm}^3$

Al -  $2,7 \text{ g/cm}^3$

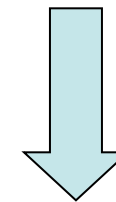
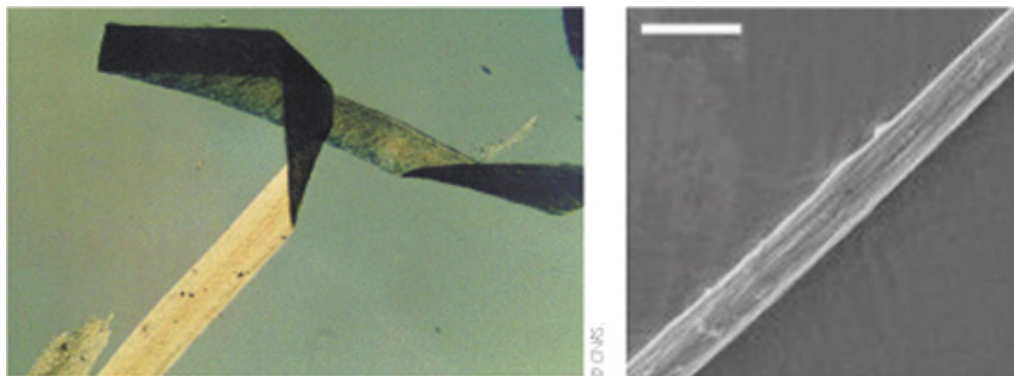
- Permitem altas tensões  $\sim 45$  billion Pa (SWCN)



Metais normais- 2 bPa!!!!



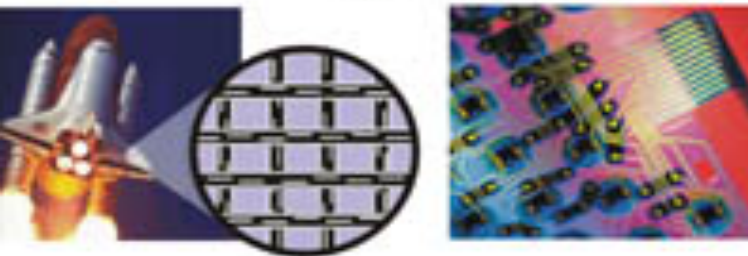
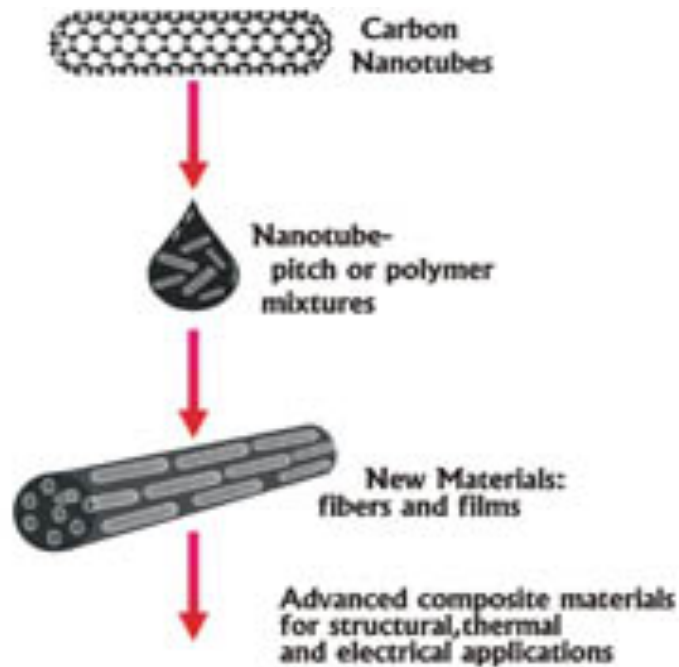
M.-F. Yu et al. Science 287, 637 (2000)



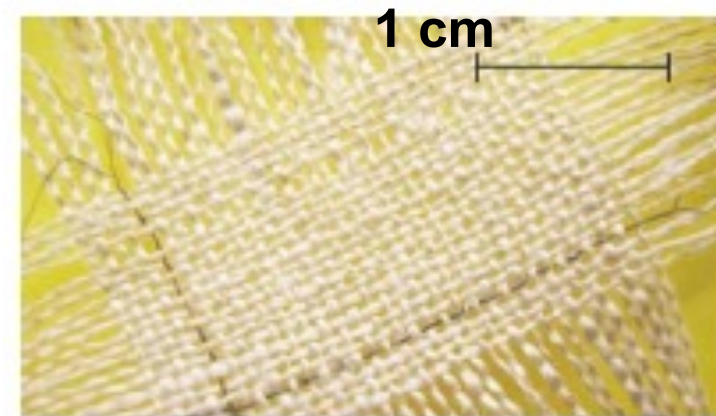
**Novas fibras de  
CNTs**



# COMPÓSITOS



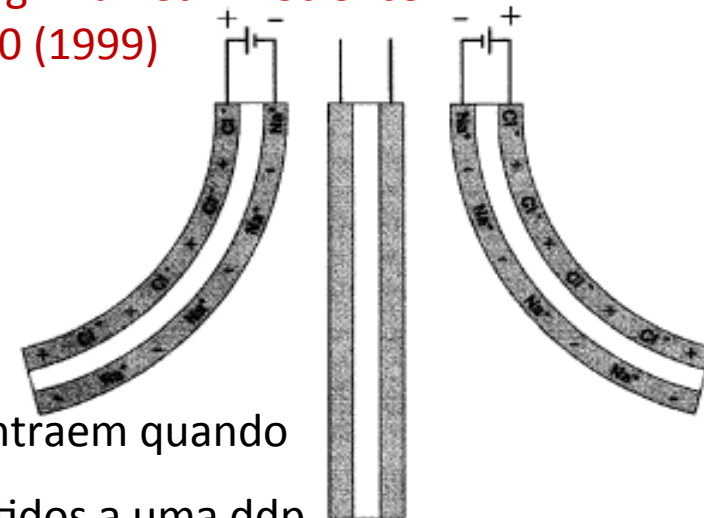
Nanotube composite materials



Science 423, 703 (2003)

## MÚSCULOS ARTIFICIAIS..

R. H. Baughman et. Al. Science 284, 1340 (1999)

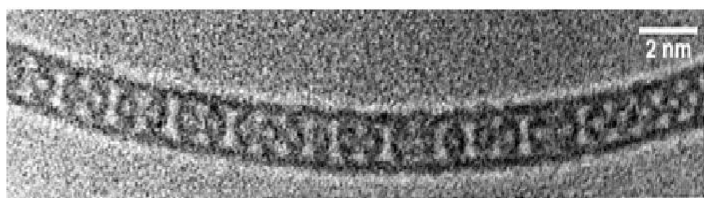
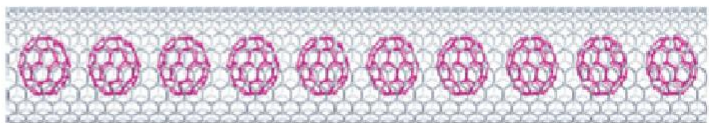


**Eletromecânica:** estendem e contraem quando submetidos a uma ddp

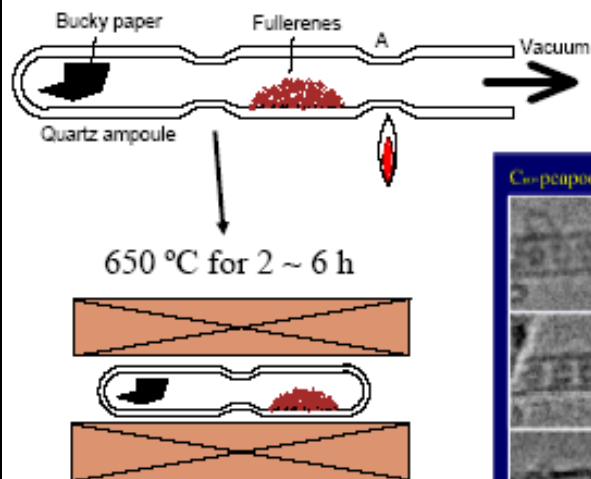




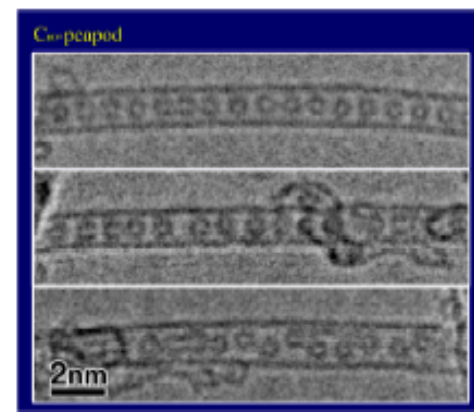
## New Materials



Fullerene  $C_{60}$  inside nanotubes



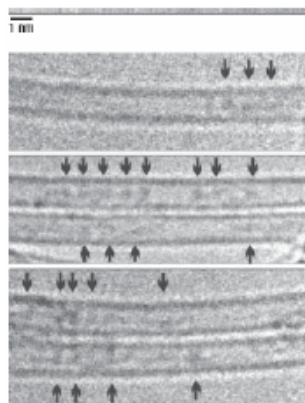
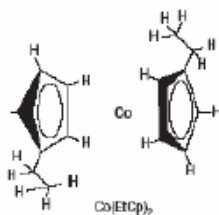
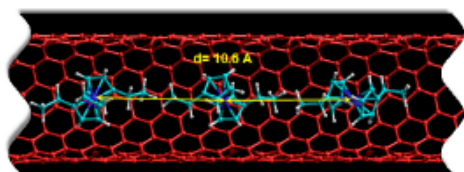
## Peapods fullerene synthesis - Kataura



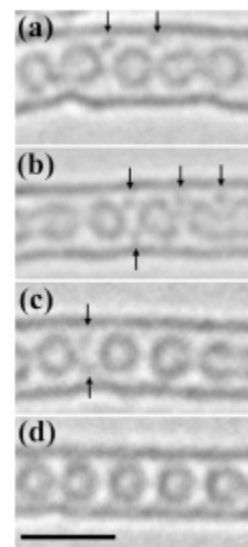
K-peapods

## Nanotubo de Carbono (10,5) Encapsulamento: CoEtCp2

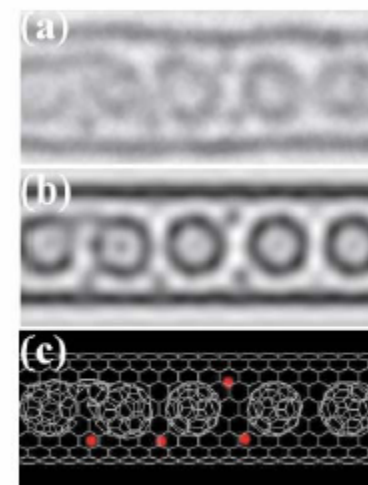
Dinâmica Molecular



Nature Materials (2005)

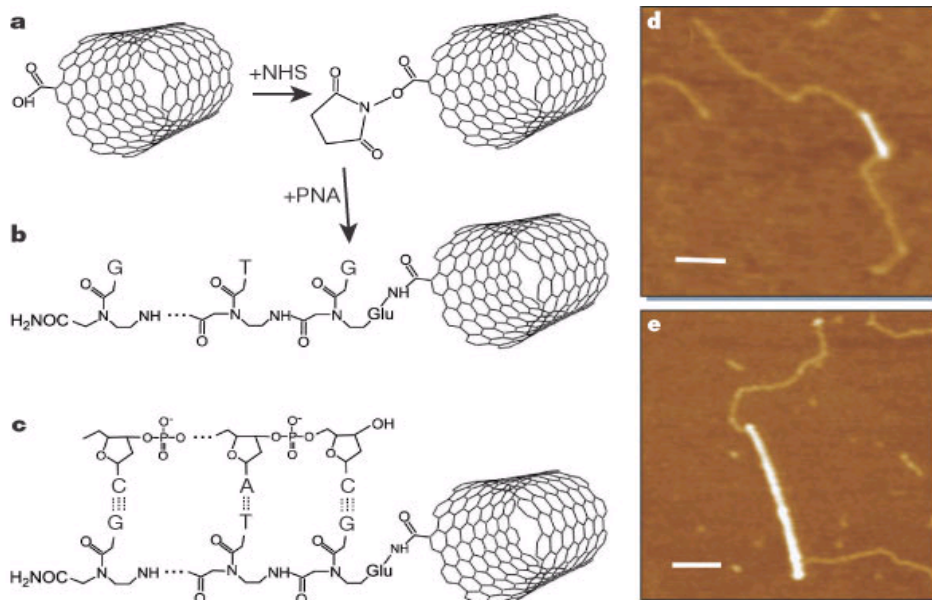


PRL 94, 045502 (2005)



# FUNCIONALIZAÇÃO DE CNTs

**Nanotechnology: Carbon nanotubes with DNA recognition**  
*Nature* **420**, 761 (2002); K. Williams, P.T.M.Veenhuizen, B G. de la Torre, R. Eritja, and C. Dekker



## Role of Defects in Single-Walled Carbon Nanotube Chemical Sensors

2006  
Vol. 6, No. 8  
1747–1751

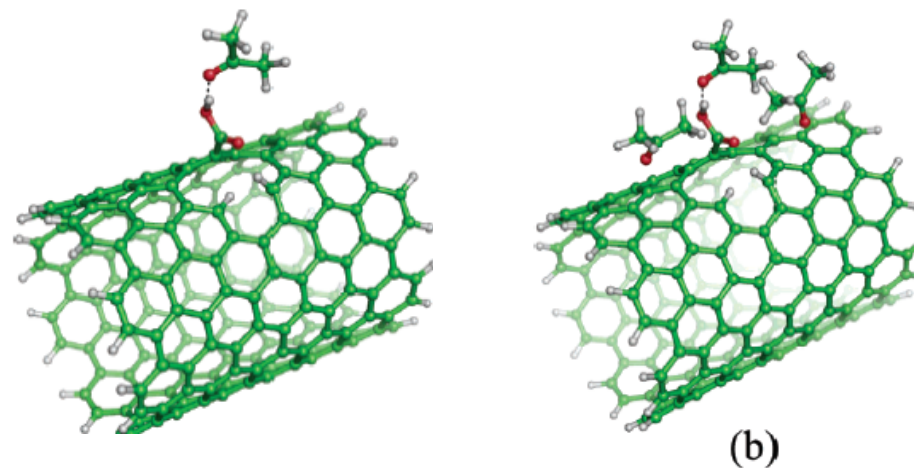
Joshua A. Robinson, Eric S. Snow,\* Ștefan C. Bădescu,  
Thomas L. Reinecke, and F. Keith Perkins

*The Naval Research Laboratory, Electronic Science and Technology Division,  
4555 Overlook Avenue, Washington, D.C. 20375*

*Received May 30, 2006; Revised Manuscript Received July 11, 2006*

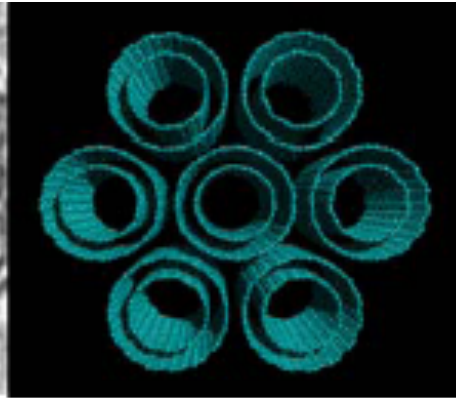
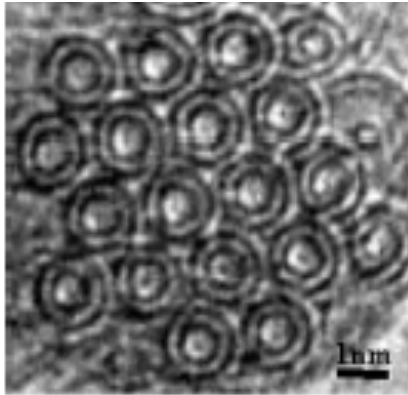
### ABSTRACT

We explore the electronic response of single-walled carbon nanotubes (SWNT) to trace levels of chemical vapors. We find adsorption at defect sites produces a large electronic response that dominates the SWNT capacitance and conductance sensitivity. This large response results from increased adsorbate binding energy and charge transfer at defect sites. Finally, we demonstrate controlled introduction of oxidation defects can be used to enhance sensitivity of a SWNT network sensor to a variety of chemical vapors.

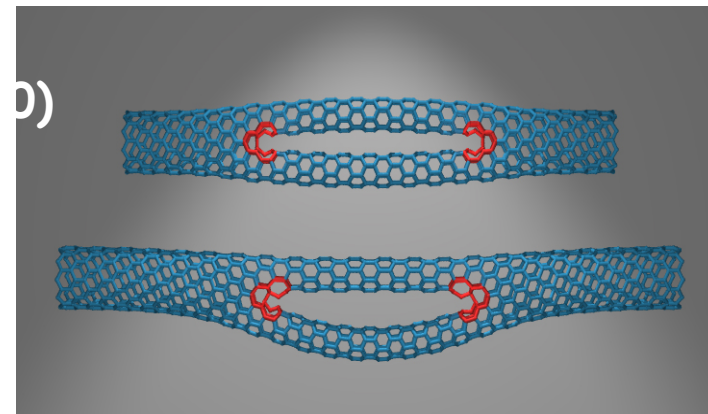
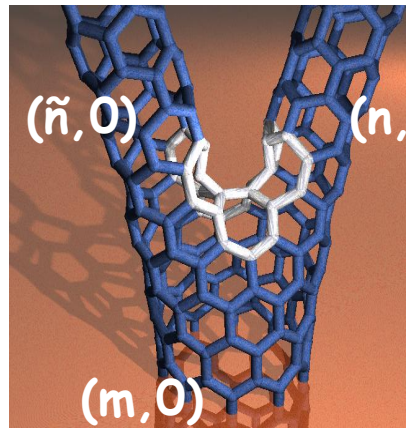


**Figure 2.** (a) Binding of acetone to a carboxylic acid defect on a SWNT sidewall. (b) Clustering of acetone around the defect via intermolecular bonding.

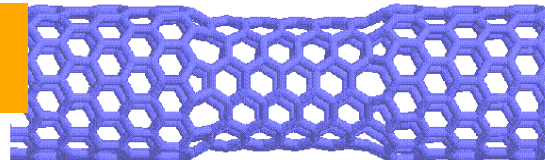
# UFF/ NANOTUBE /ZOO



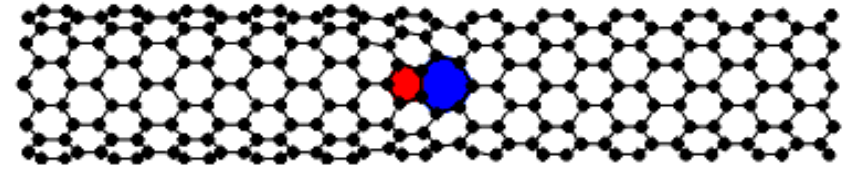
Nanotubos de Parede duplas  
(Double wall nanotube)



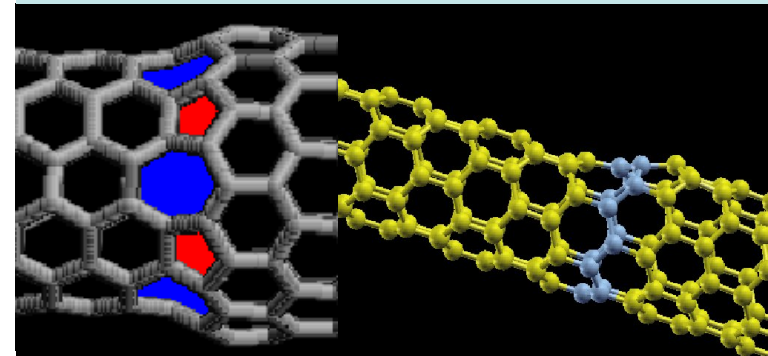
## Y-JUNÇÕES E Y-ANÉIS



## NANOESTRUTURAS DE CNTS



## Defeito Topológico (n,0)/(n-1,0)



## QUANTUM DOTS

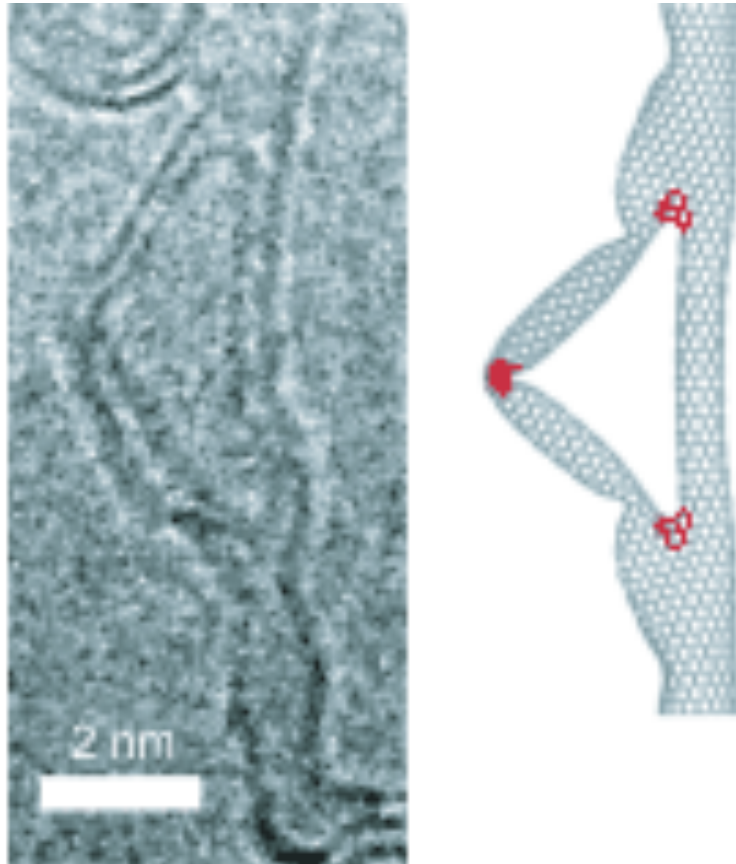




Communication

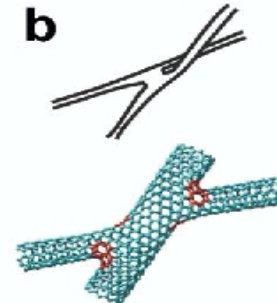
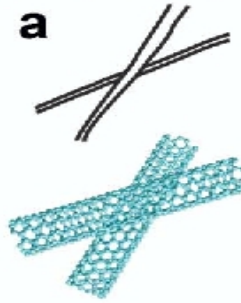
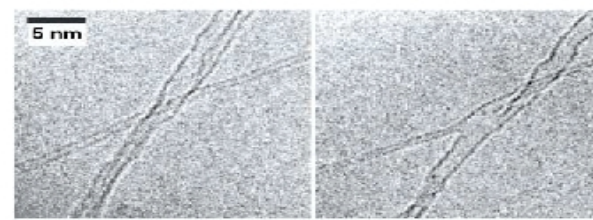
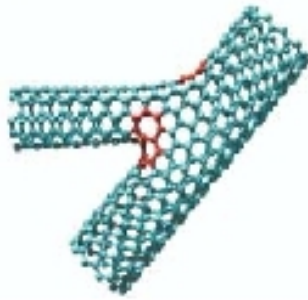
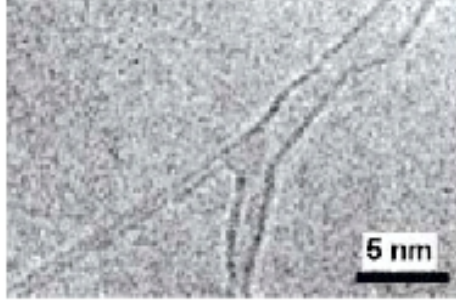
Synthesis of SWCNT Rings Made by Two Y Junctions and Possible Applications in Electron Interferometry†

Authors **Daniel Grimm**, Pedro Venezuela Prof., Florian Banhart Prof., Nicole Grobert Dr., Humberto Terrones Prof., Pulickel M. Ajayan Prof., Mauricio Terrones Prof.,  
**Andrea Latgé Prof.**



The formation of ringlike junction structures made from single-walled carbon nanotubes has been observed by transmission electron microscopy (see image). A merging process of asymmetric into symmetric rings using carbon nanotubes was investigated under electron-beam irradiation at high temperatures. Based upon these observations, a rich variety of tailor-made double-slit interferometers with defined ring symmetries can be realized

# Y-JUNCTIONS & RINGS

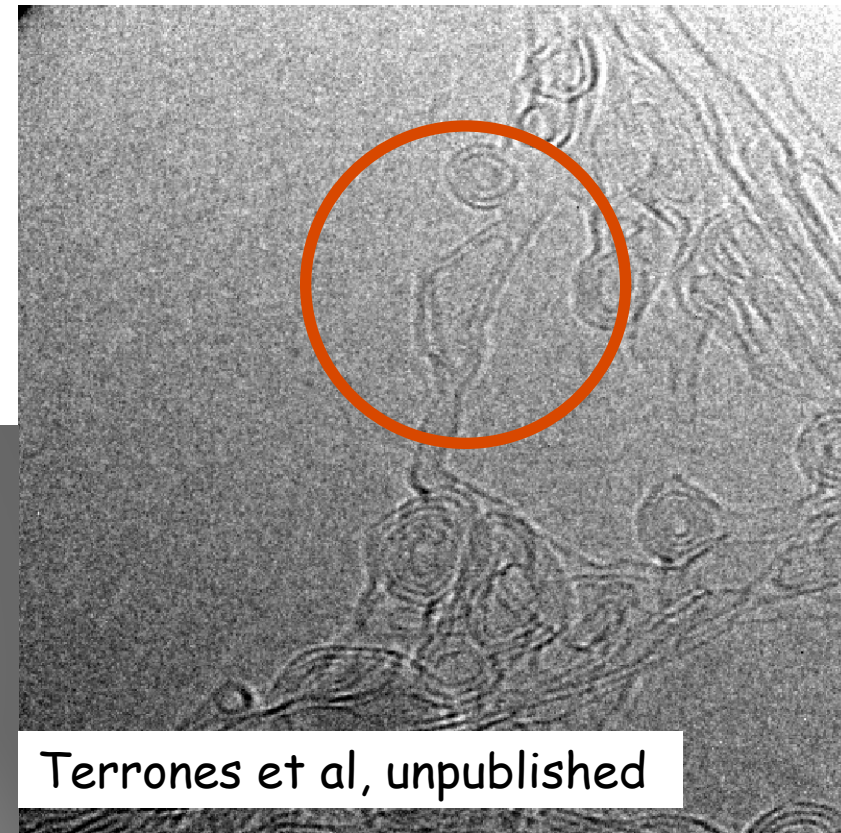
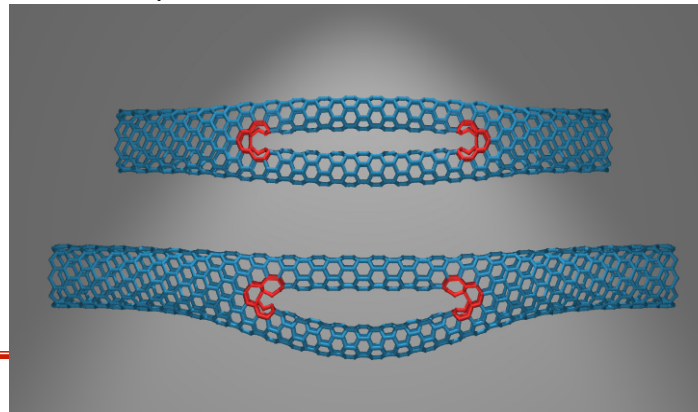


CN  
ZOO

CN Junctions, X, Y e T- synthesized via electron beam exposure in nanotubes controlled at high temperatures (800° C) [high-temperature electron beam]  
M. Terrones, PRL 89 75505 (2002)

## YJ -Electronic and transport Stability

A. Latge et al, PRB & Chem. Phys. A (2005)

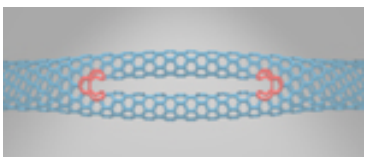


Terrones et al, unpublished

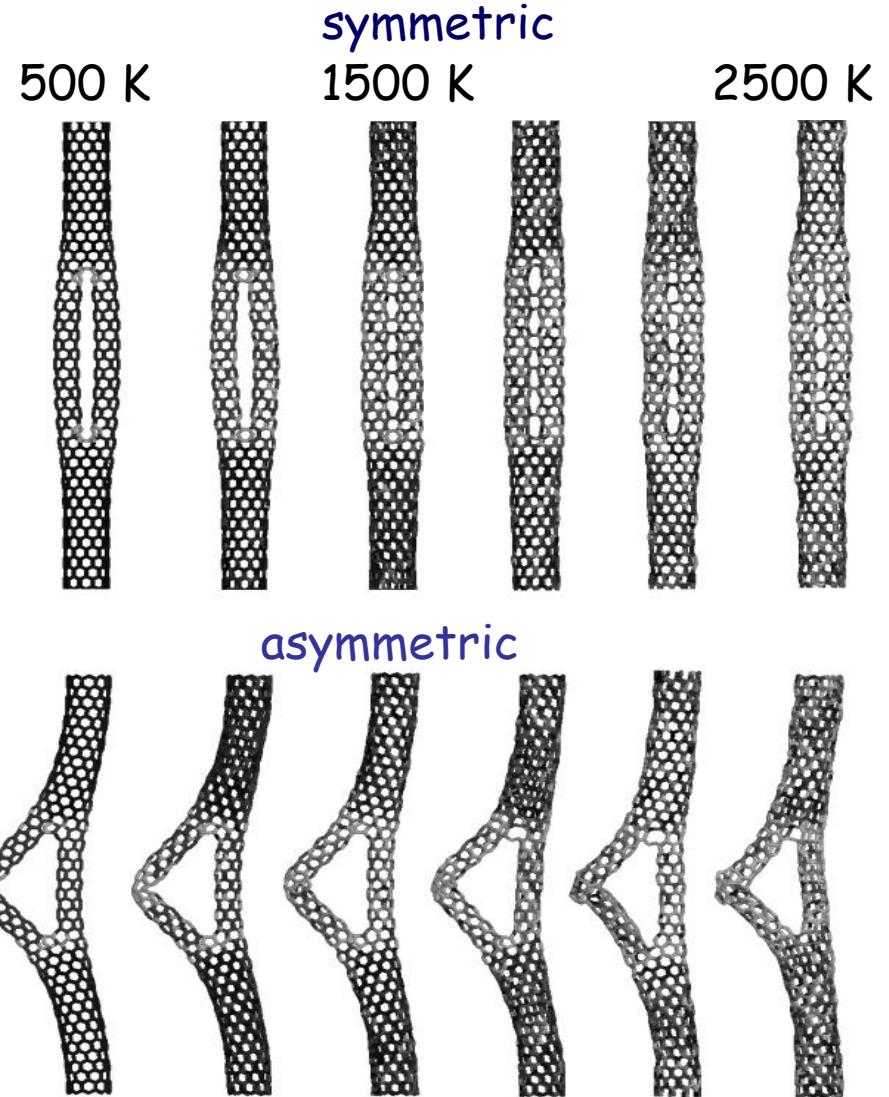
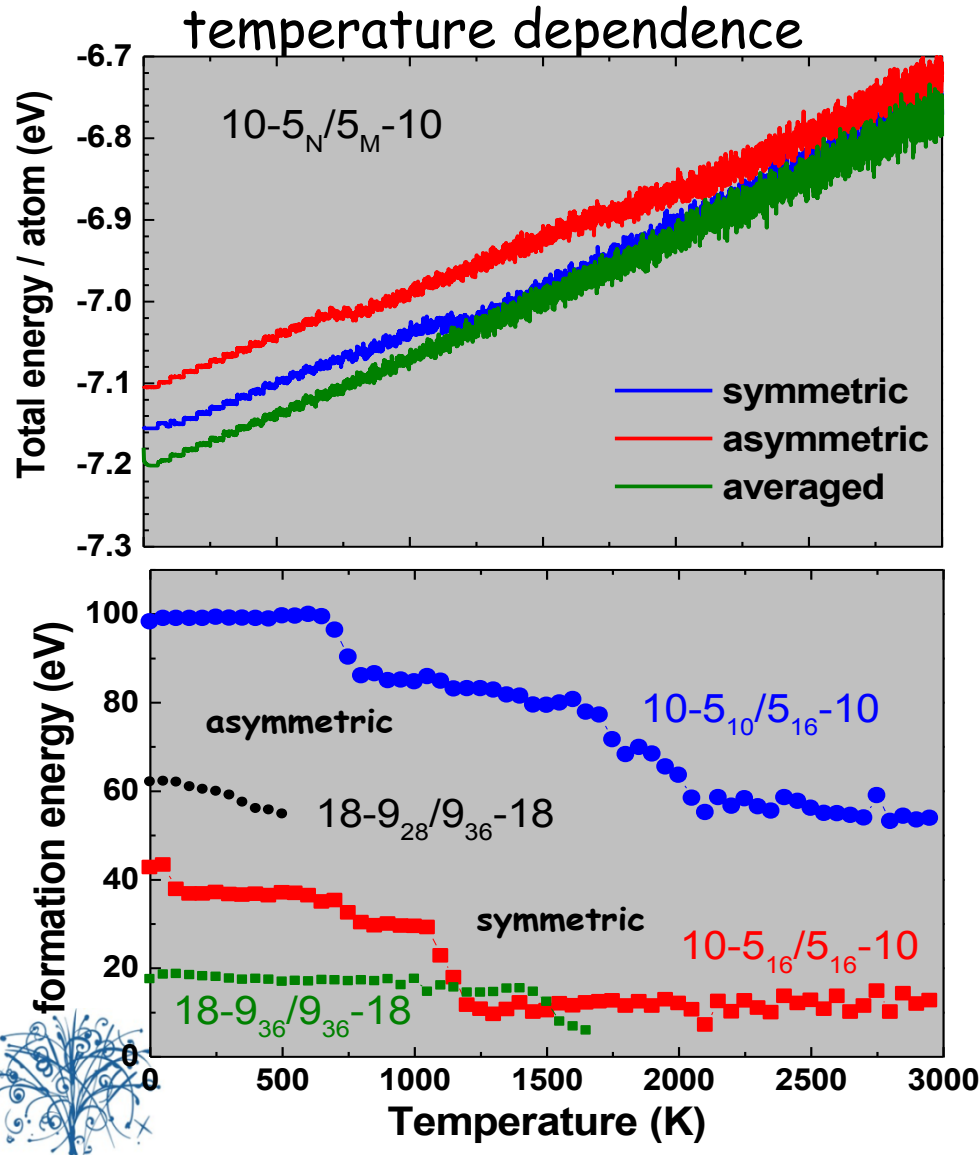




# Stability: Y-ring



Monte Carlo Simulation  
Metropolis - Tersoff Potential



A. Latgé et al, PRB & Chem. Phys. A (2005)



NT07

# Eighth International Conference on the Science and Application of Nanotubes

24 - 29 June 2007

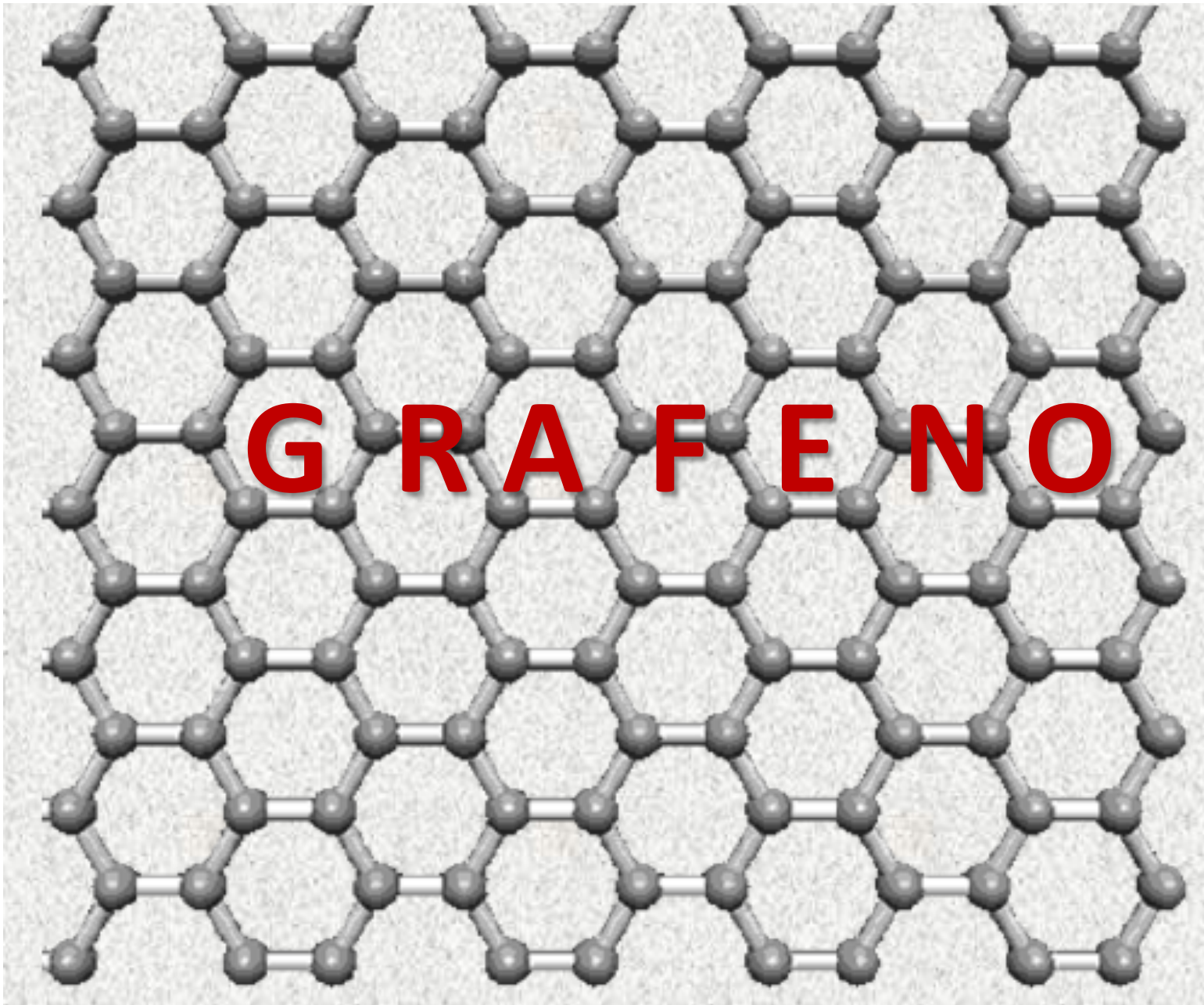
Parque Metalúrgico - Centro de Artes e Convenções - Ouro Preto - Minas Gerais - Brazil



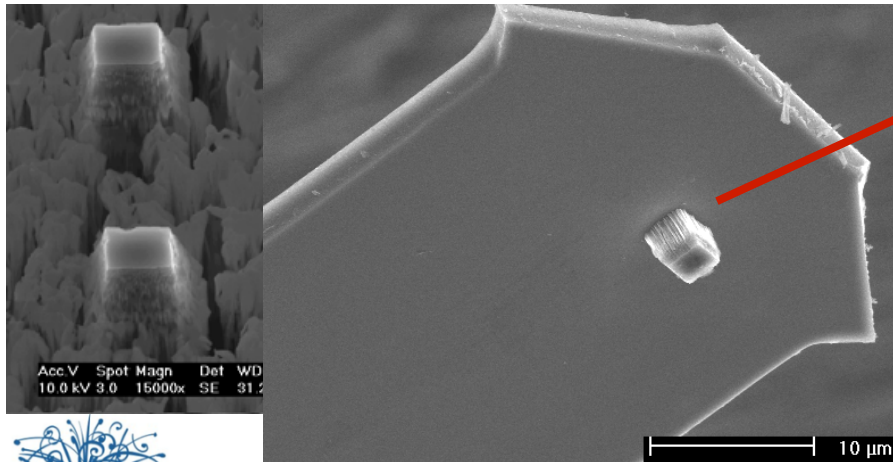
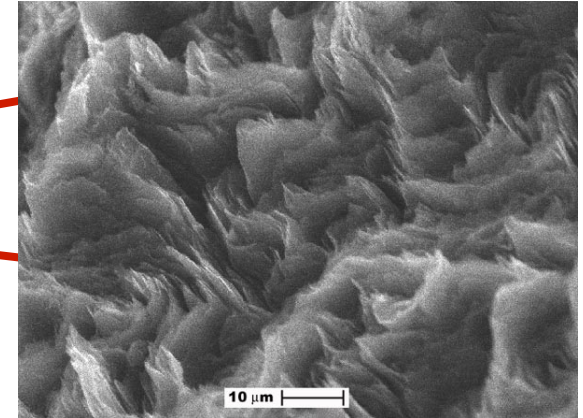
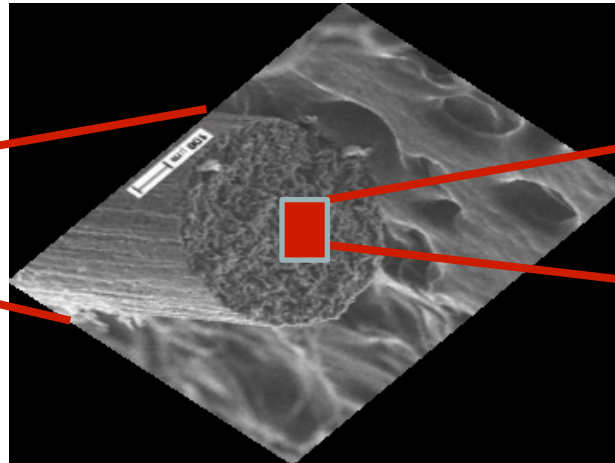
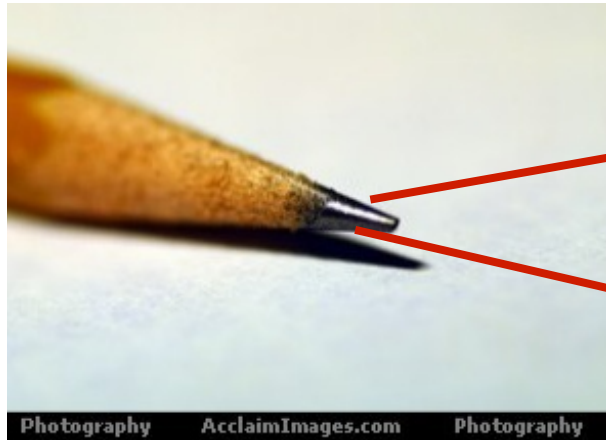
INCT

Instituto Nacional de Ciência e Tecnologia em  
**Nanomateriais de Carbono**





# TENTANDO OBTER GRAFENO



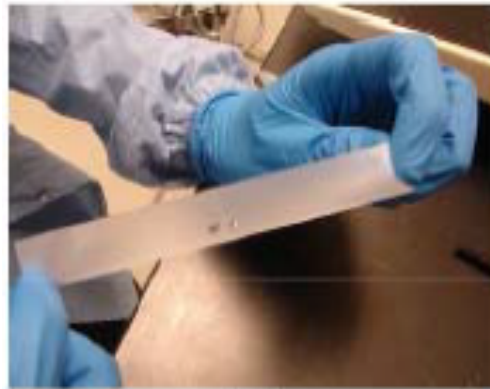
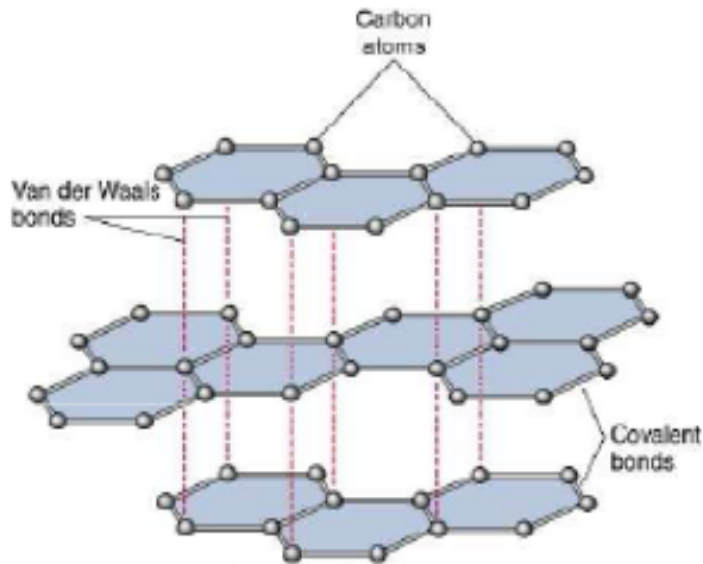
**GRAFENO  
MICROCRISTAL**





# EXFOLIAÇÃO MECÂNICA DO GRAFITE

## Scotch Tape Method



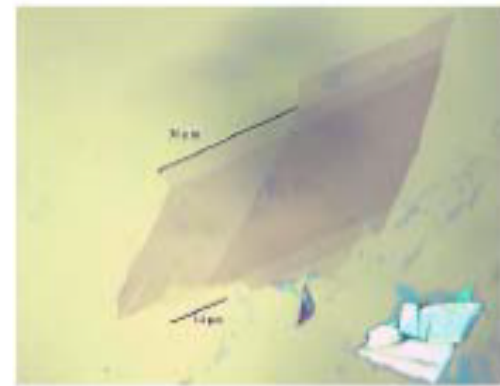
(1)



(2)



(3)



(4)

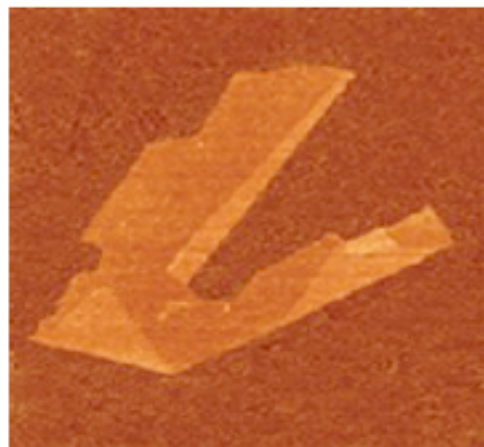
**VANTAGENS: SIMPLES E FÁCIL**  
**ALTA QUALIDADE**

**DESVANTAGENS: BAIXA EFICIÊNCIA**

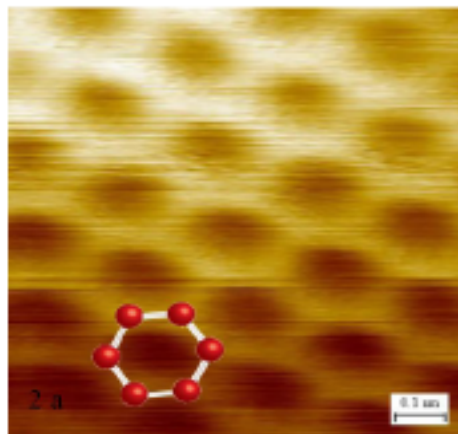


# “the Scotch tape method.”

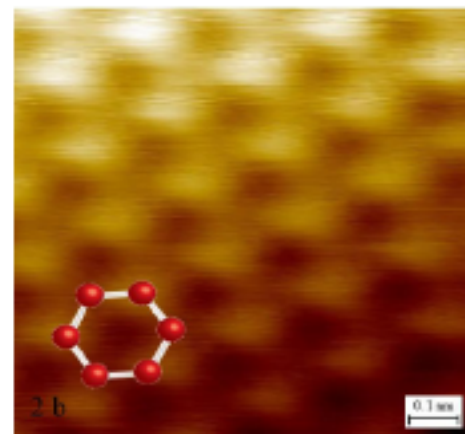
Single graphene sheets can be isolated by repeated cleavage of graphite crystals (“exfoliation”).



AFM image (Geim et al.)  
(Single layer flake on SiO<sub>2</sub> substrate)



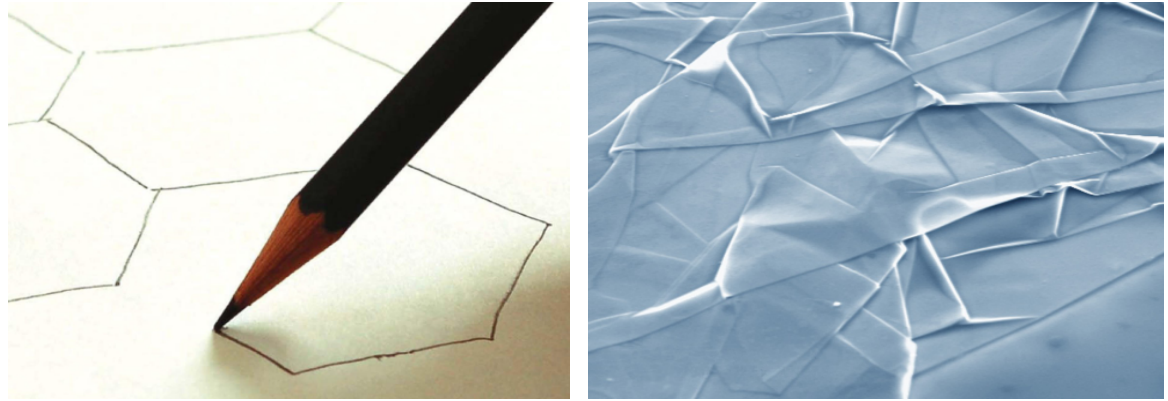
STM image (Stolyarova et al.)



- Novoselov *et al.* Science '04, Nature '05
- Zhang *et al.*, Nature '05

➡ 1564: INVENÇÃO do “Lead pencil” baseado no GRAFITE

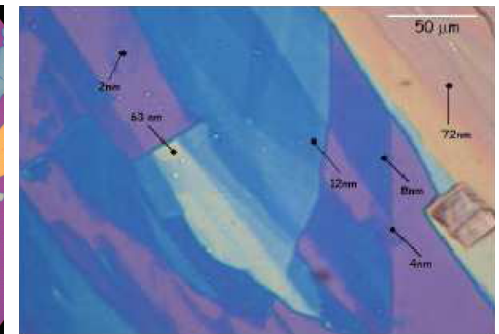
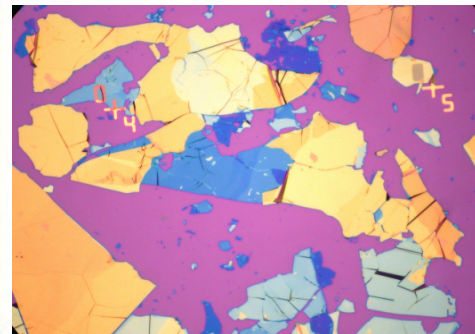
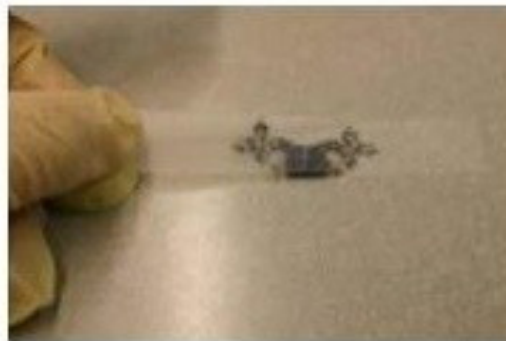
GRAFENO



➡ 1946 P.R. Wallace - paper sobre estrutura de banda de grafeno

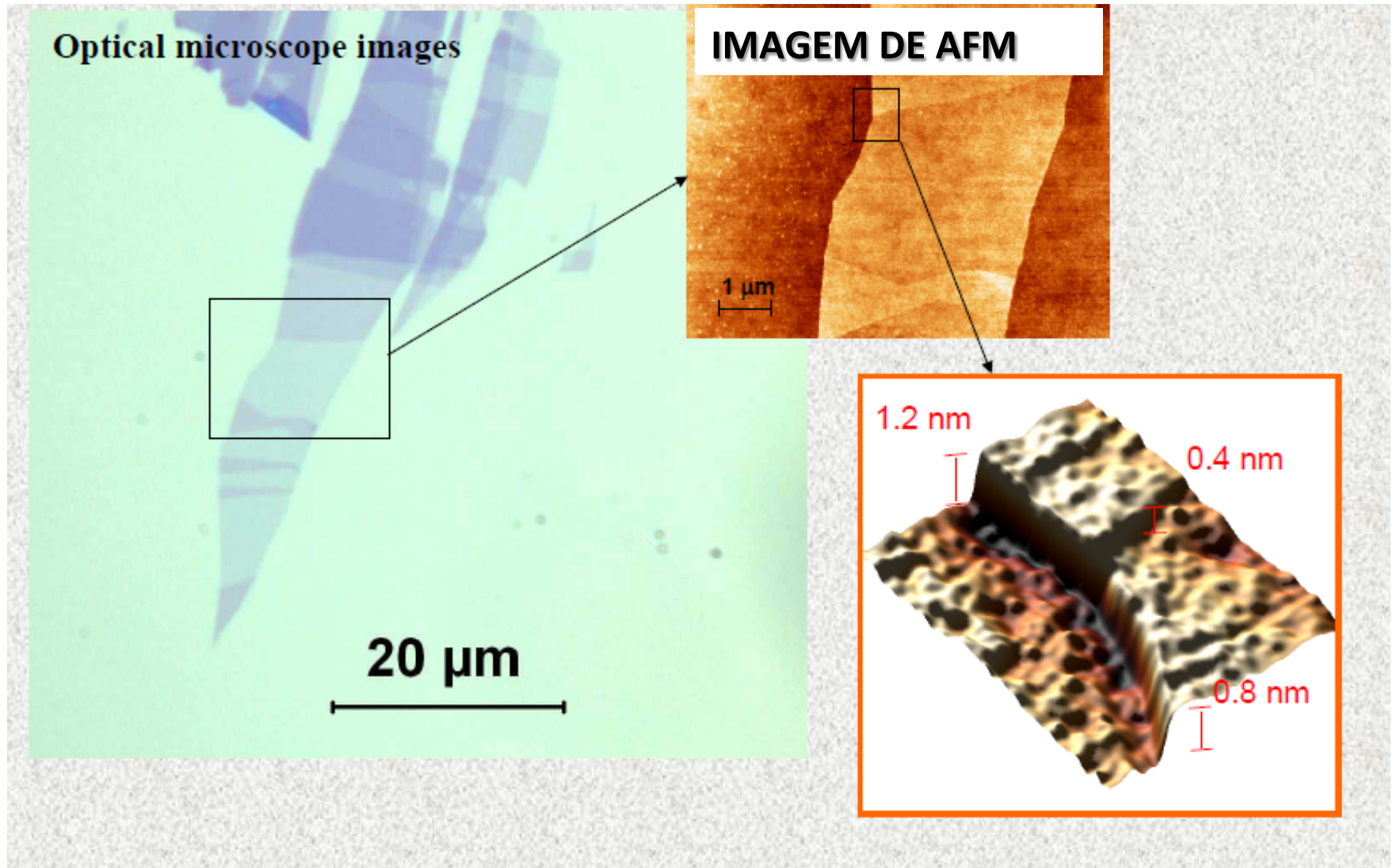
➡ 2004 K.S. Novoselov & A. Geim realizam e identificam o grafeno exper.

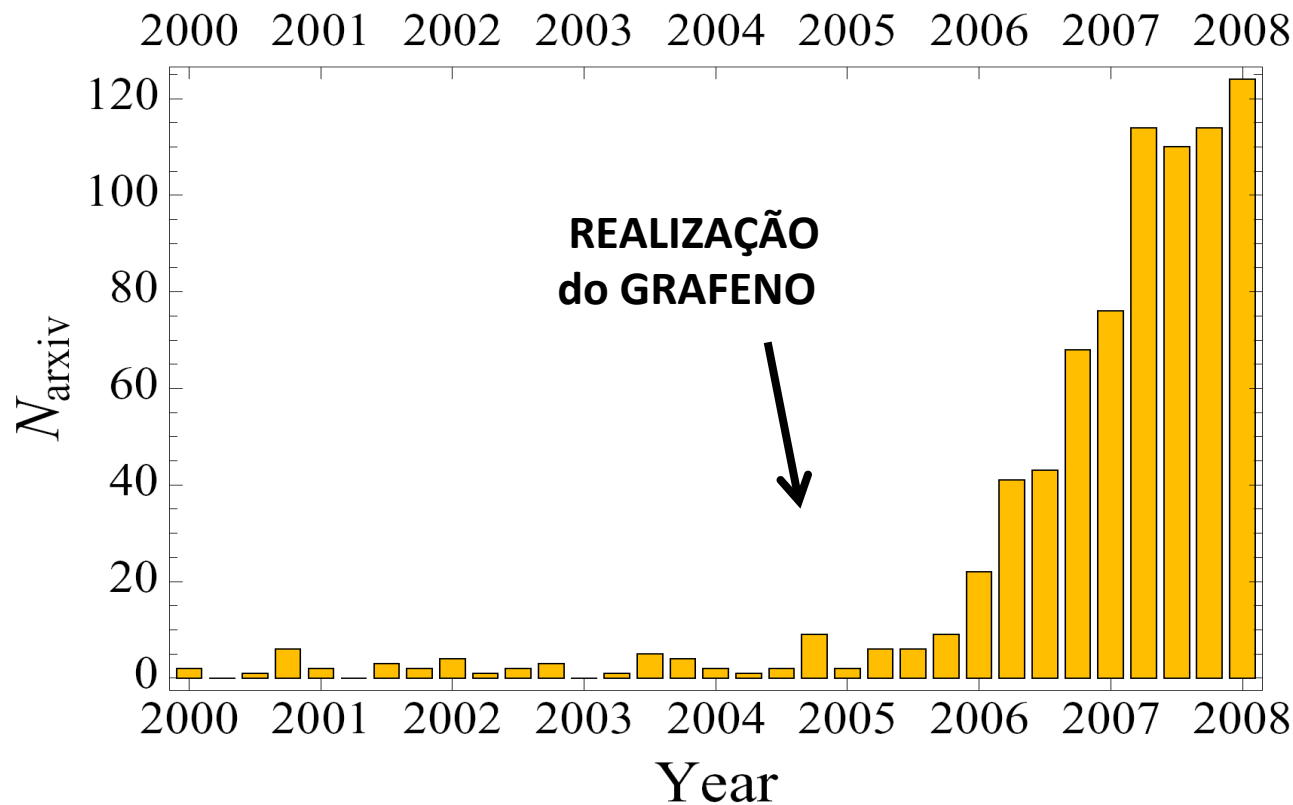
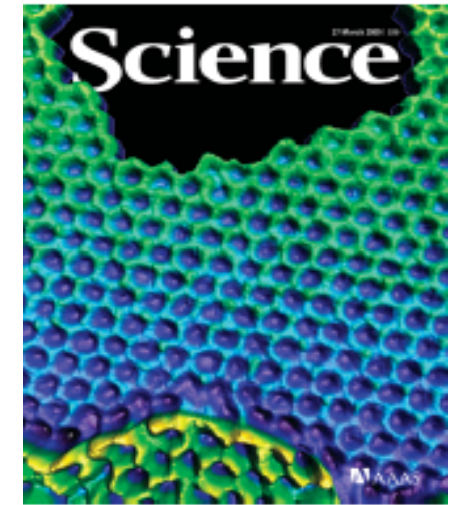
Wafer with graphene flakes, optical microscope  
(Novoselov et al.,  
Science 306, 666  
(2004))





# ALGUMAS CAMADAS DE GRAFENO SOBRE SUBSTRATO DE $\text{SiO}_2/\text{Si}$





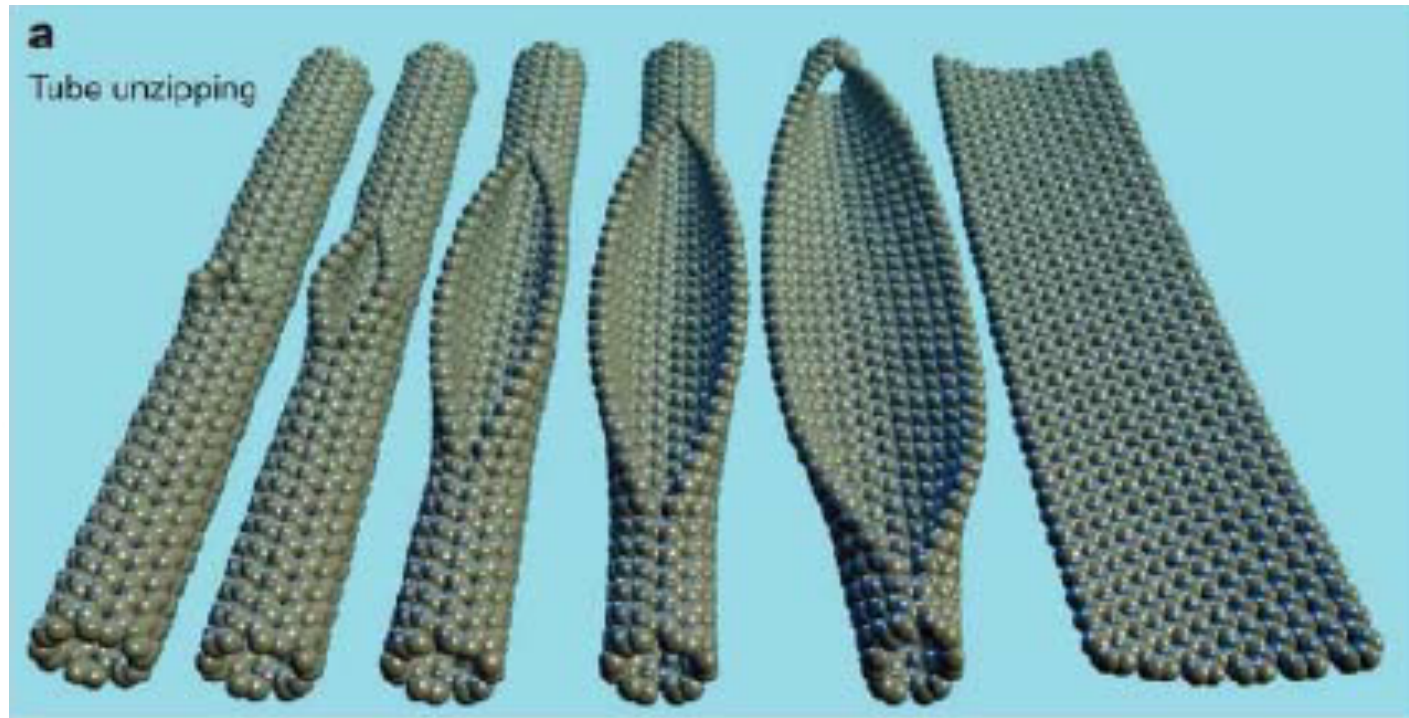
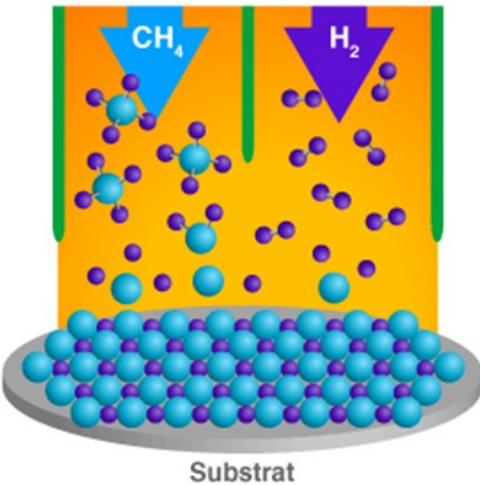
**ANDRE GEIM  
&  
NOVOSELOV**

**NOBEL PHYSICS  
PRIZE 2010**

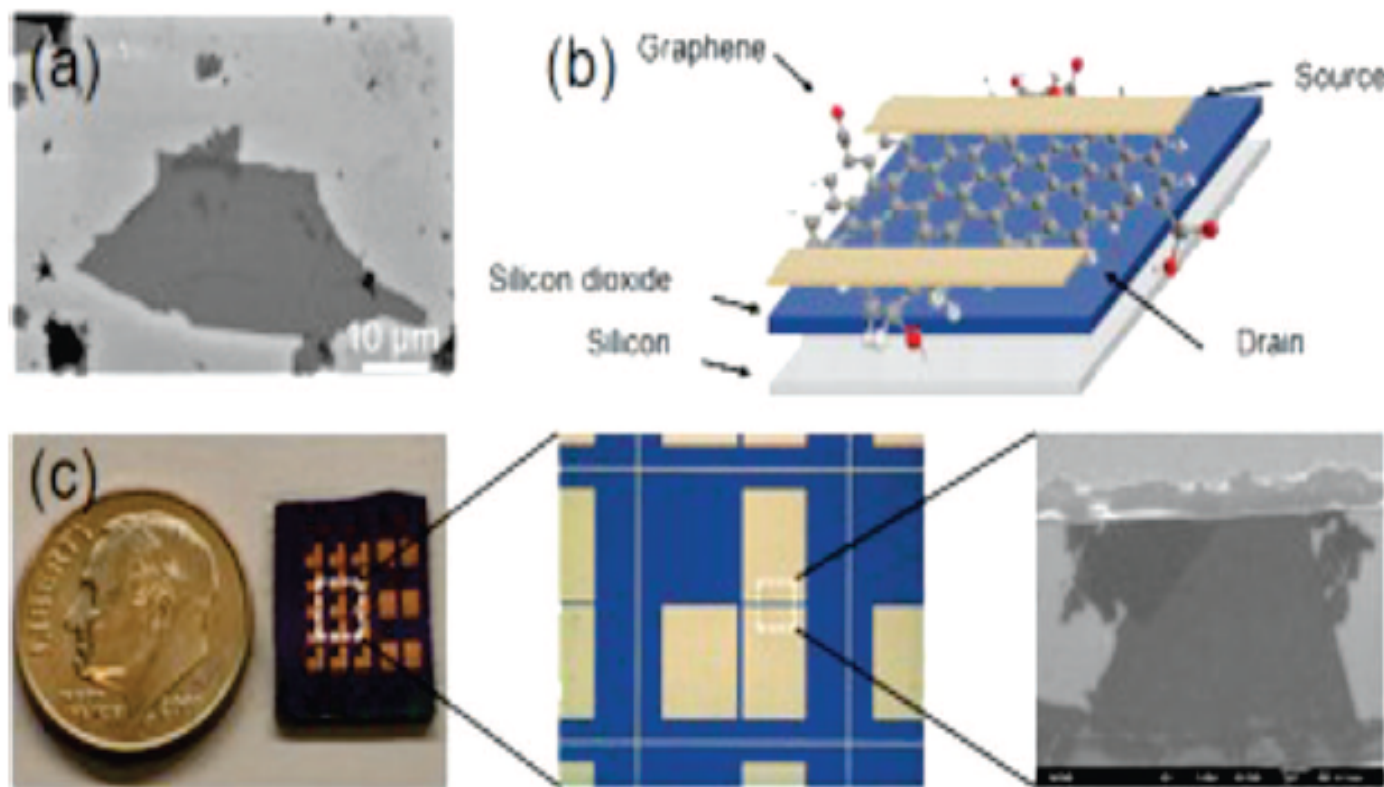
# OUTRAS FORMAS DE SE FAZER GRAFENO:

- Rotas químicas
- Depositar em SiC
- Deposição química a vapor
- CNTs – processos de unzip

Chemical Vapor Deposition (CVD)



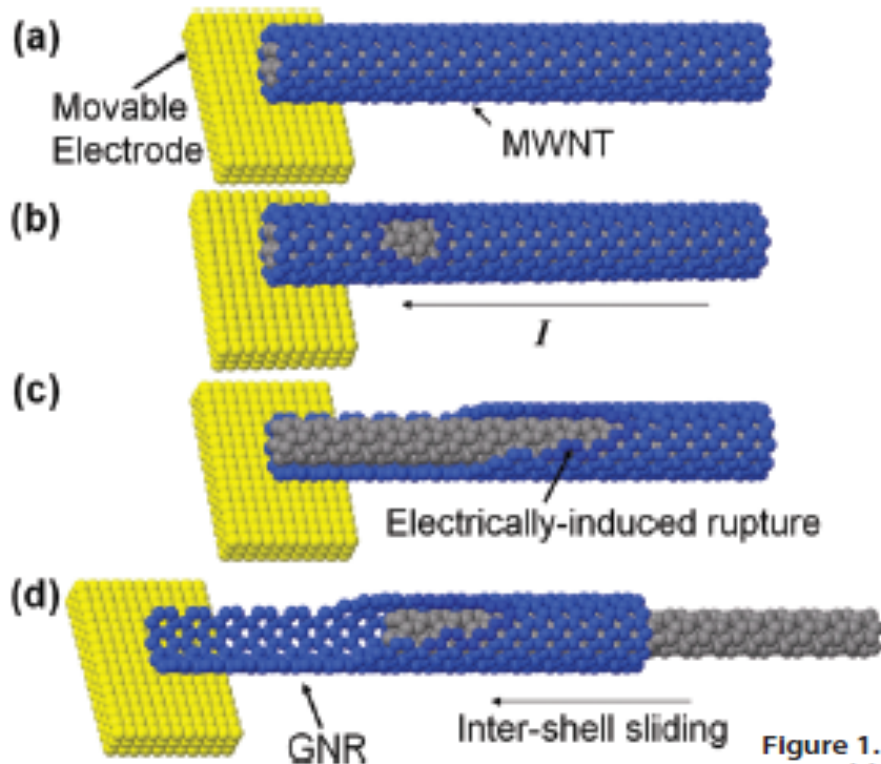




**Figure 15.** (a) SEM image of a large single sheet deposited on SiO<sub>2</sub>. (b) Schematic view of a top-contact, back-gated device. (c) Photograph (left), optical image (middle), and SEM image (right) of a working device with a channel length of 7 μm. (Reprinted with permission from ref 101. Copyright 2009 Nature Publishing Group.)



# NANOFITAS de GRAFENO

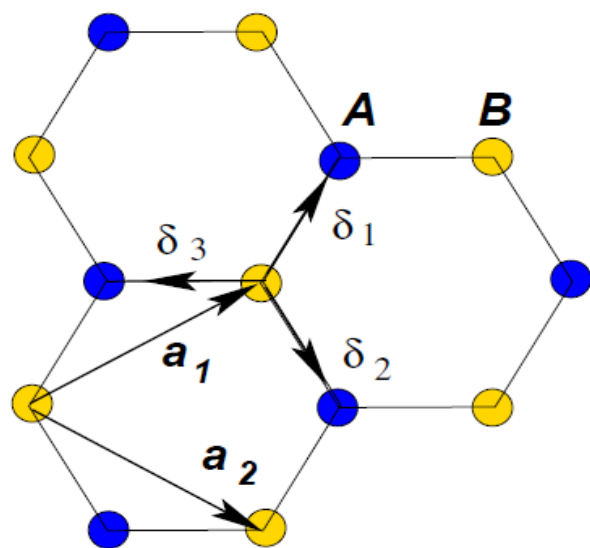


NANOFITAS A  
PARTIR DE  
NANOTUBOS DE  
CARBONO

Figure 1. Schematic drawings of the proposed graphene nanoribbon (GNR) fabrication from a multiwall carbon nanotube (MWNT). In the schematic, a double-wall carbon nanotube (DWNT) is chosen for simplicity: (a) MWNT before the partial wall rupture; (b) electrical current induces rupture of the outer wall of a MWNT; (c) partial outer-wall rupture of a MWNT results in a precursor GNR which is under the MWNT inner core; (d) Intershell sliding between the GNR and the inner core results in a suspended, electrically contacted GNR.



# GRAFENO: CÉLULA UNITÁRIA



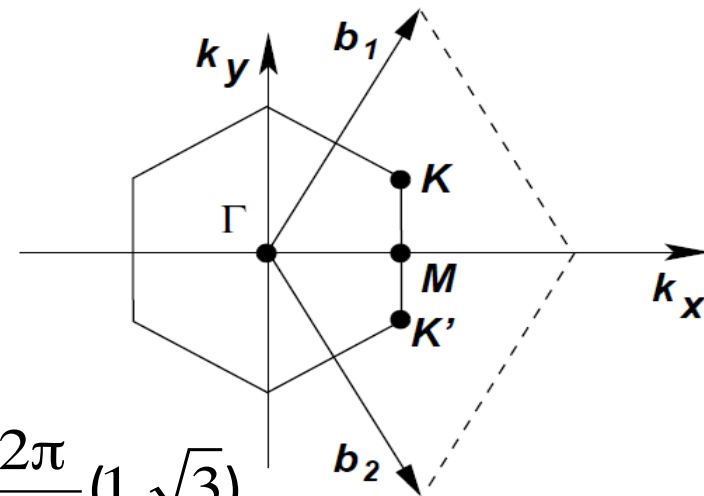
$$\mathbf{r}_{a_1} = \frac{a_{cc}}{2} (3, \sqrt{3})$$

$$\mathbf{r}_{a_2} = \frac{a_{cc}}{2} (3, -\sqrt{3})$$

$$a_{cc} : 1.42 \text{ \AA}$$

$$\mathbf{r}_{b_1} = \frac{2\pi}{3a_{cc}} (1, \sqrt{3})$$

$$\mathbf{r}_{b_2} = \frac{2\pi}{3a_{cc}} (1, -\sqrt{3})$$



DIRAC POINTS: **K & K'**

$$\mathbf{r}_K = \frac{2\pi}{3a_{cc}} (1, \frac{1}{\sqrt{3}}) \quad \mathbf{r}_{K'} = \frac{2\pi}{3a_{cc}} (1, -\frac{1}{\sqrt{3}})$$

VIZINHOS: 3 primeiros vizinhos

$$\mathbf{r}_{\delta_1} = \frac{a_{cc}}{2} (1, \sqrt{3}) \quad \mathbf{r}_{\delta_2} = \frac{a_{cc}}{2} (1, -\sqrt{3}) \quad \mathbf{r}_{\delta_3} = -a_{cc} (1, 0)$$

6 segundos vizinhos

$$\mathbf{r}_{\delta_1'} = \pm \mathbf{a}_1 \quad \mathbf{r}_{\delta_2'} = \pm \mathbf{a}_2 \quad \mathbf{r}_{\delta_3'} = \pm (\mathbf{a}_2 - \mathbf{a}_1)$$





$$H = -t \sum_{\langle i,j \rangle} (a_{i\sigma}^\dagger b_{j\sigma} + hc) - t_1 \sum_{\langle\langle i,j \rangle\rangle} (a_{i\sigma}^\dagger a_{j\sigma} + b_{i\sigma}^\dagger b_{j\sigma} + hc) - t_2 \sum_{\langle\langle\langle i,j \rangle\rangle\rangle} (a_{i\sigma}^\dagger b_{j\sigma} + hc)$$

A função de onda que descreve as bandas  $p_z$  ( $\pi$ ) podem ser escritas como:

$$\Psi_{k,s}(r) = \frac{1}{\sqrt{N}} e^{ikR} [\alpha_{k,s} \phi_A(R) + \beta_{k,s} \phi_B(R)]$$

Resolver um determinante secular

$$\begin{vmatrix} H_{AA} - ES & H_{AB} \\ H_{BA} & H_{BB} - ES \end{vmatrix} = 0$$

$$E = \frac{1}{2} [H'_{AA} + H'_{BB} \pm ((H'_{AA} - H'_{BB})^2 + 4 |H'_{AB}|^2)^{1/2}]$$

$$E = H'_{AA} \pm |H'_{AB}|; \quad H'_{AA} = H_{AA} / N;$$

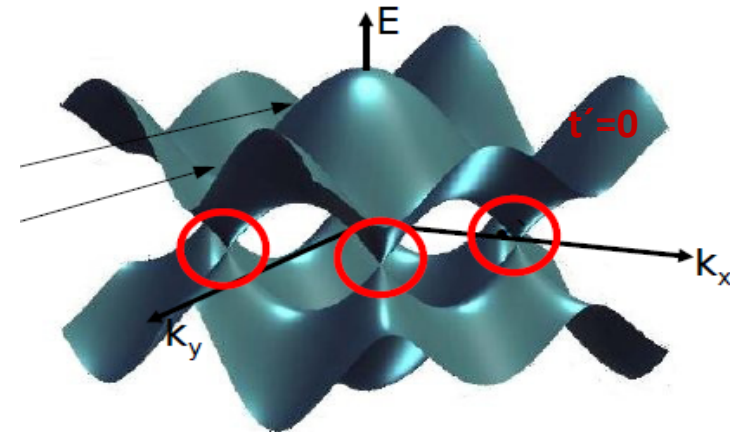
$$H_{AB} = -t \sum_j e^{ik \cdot \delta_j}$$

$$H\Psi_k(r) = E\Psi_k(r)$$

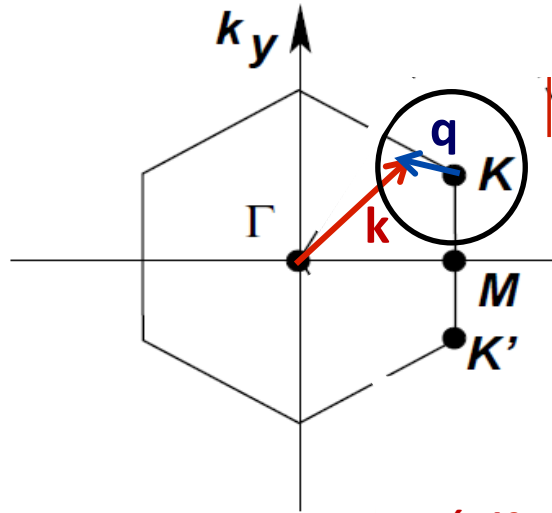
$$S = \int \phi_A^* \phi_A d\tau = \int \phi_B^* \phi_B d\tau$$

$$H_{AA(BB)} = \int \phi_{A(B)}^* H \phi_{A(B)} d\tau$$

$$H_{AB(BA)} = \int \phi_{B(A)}^* H \phi_{A(B)} d\tau$$



Expansão:  $\mathbf{k}=\mathbf{K}+\mathbf{q}$   $|\mathbf{q}| \ll |\mathbf{K}|$



$$f(\mathbf{K} + \mathbf{q}) = 2 \cos(\sqrt{3}(K_y + q_y)a_{cc}) + 4 \cos\left(\frac{3}{2}(K_x + q_x)a_{cc}\right) \cdot \cos\left(\frac{\sqrt{3}}{2}(K_y + q_y)a_{cc}\right)$$

using:  $\cos(\sqrt{3}q_y a) \approx 1 - \frac{3q_y^2 a^2}{2}$  and  $K_x = \frac{2\pi}{3a_{cc}}; K_y = \frac{2\pi}{3\sqrt{3}a_{cc}}$

$$f(\mathbf{K} + \mathbf{q}) = -3 + \frac{9q^2 a_{cc}^2}{4}$$

$$v_F = \frac{3ta_{cc}}{2h} \approx \frac{c}{300} \approx 10^6 \text{ m/s}$$

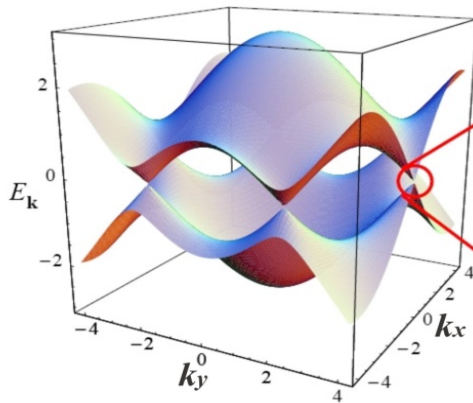
até 1ª viz

até 2ª viz

$$E_{\pm}(\mathbf{q}) \approx v_F |\mathbf{q}| + O\left(\frac{q}{K}\right)^2$$

$$E_{\pm}(\mathbf{q}) \approx 3t' \pm v_F |\mathbf{q}| - \left( \frac{9t'a_{cc}^2}{4} \pm \frac{3ta_{cc}^2}{8} \sin(3\theta_q) \right) |\mathbf{q}|^2$$

$$\theta_q = \arctan\left(\frac{q_x}{q_y}\right)$$

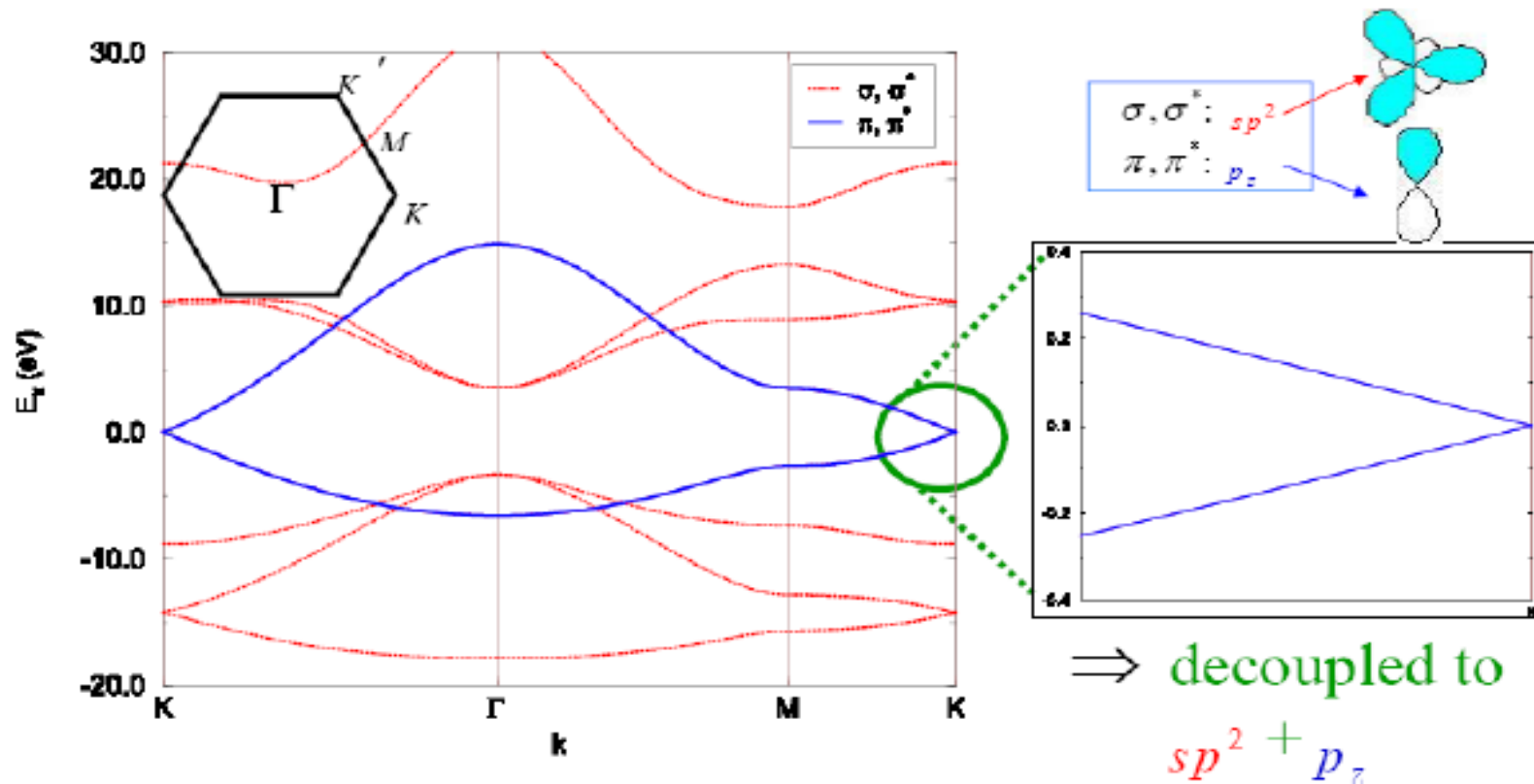


Relação linear energia

Mapeamento do problema num quadro relativístico de partícula sem massa descrito pela equação de Dirac para spins 1/2



# ESTRUTURA DE BANDA DO GRAFENO

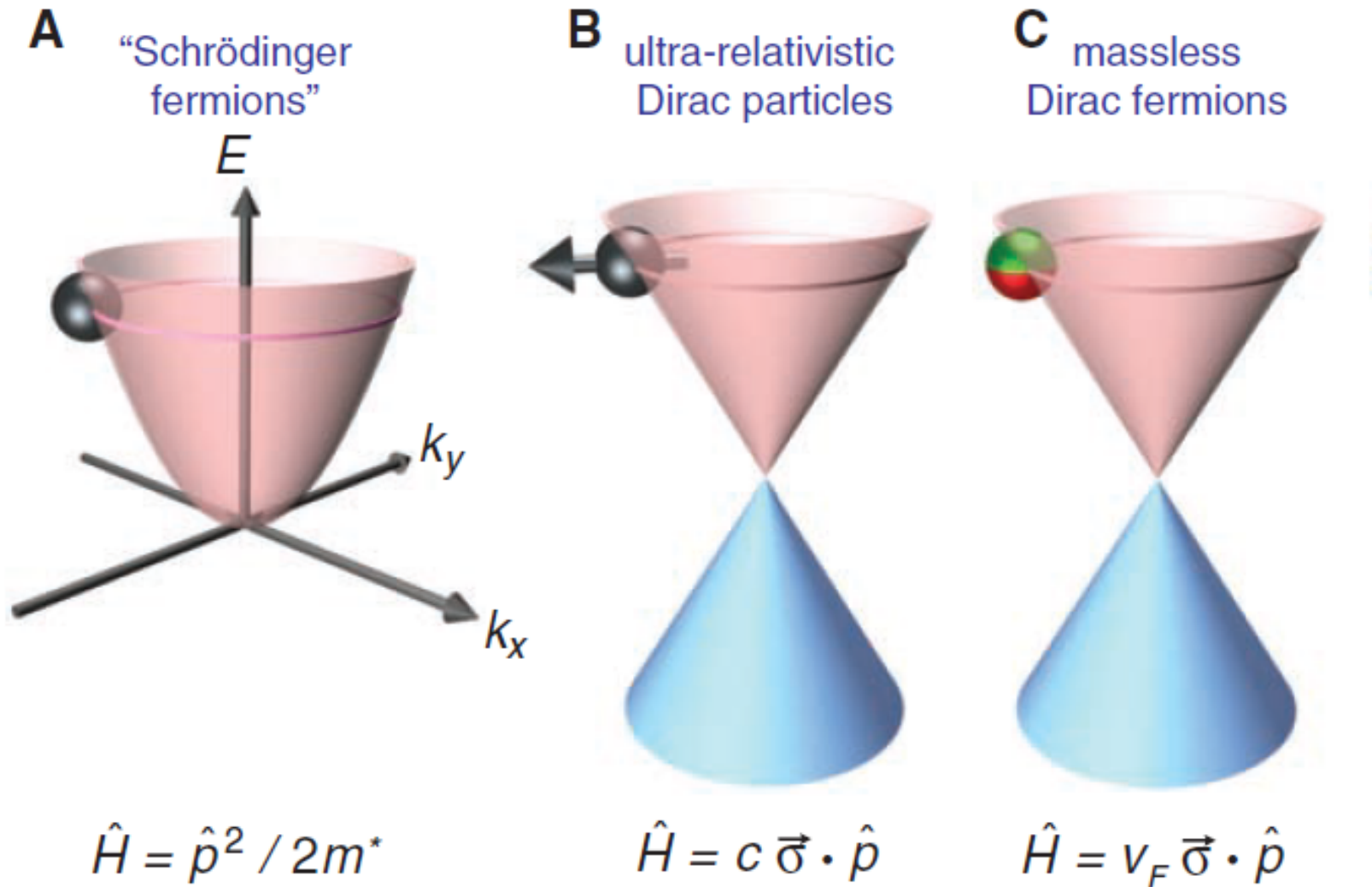


➡ Comparando a estrutura de banda de modelos DFT e TB se conclui que a estrutura de banda consiste em bandas desacopladas  $sp^2$  and  $p_z$





# ZOOLOGICO DAS QUASIPARTICULAS



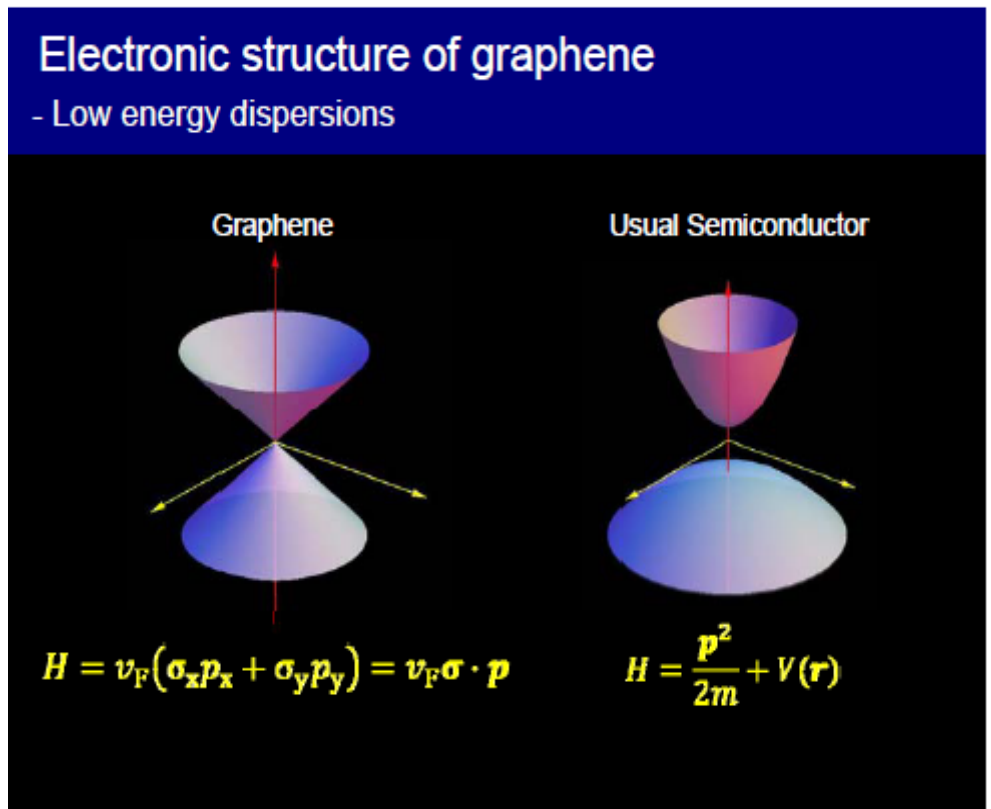
$$E(k) = \hbar v_F |k|$$

- No gap
- DOS  $(\partial N / \partial E) \approx E$
- Dois vales
- Função de onda spinor (A,B)

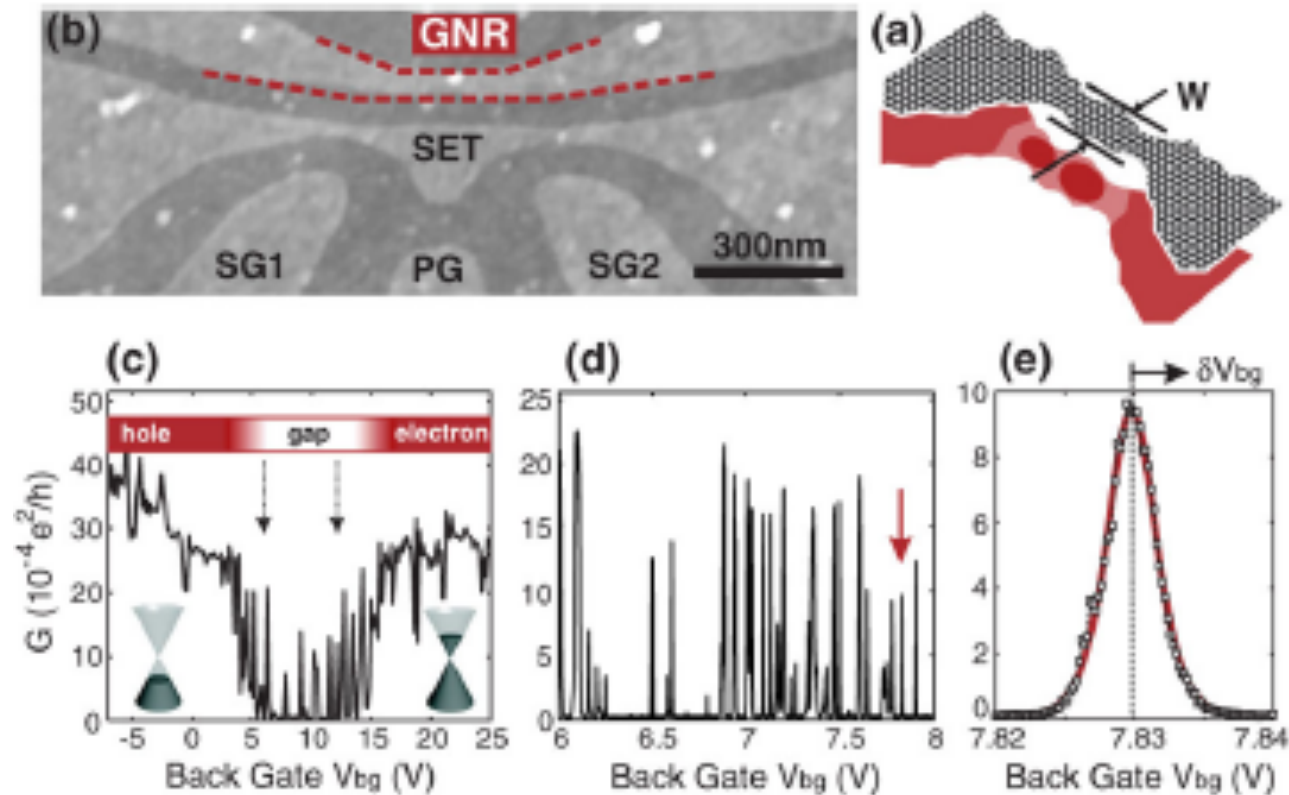
$$E(k) = \frac{\hbar^2 k^2}{2m^*}$$

- Gap 1.5 eV GaAS
- DOS(E)=const
- Autofunções ondas planas

# GRAFENO X SEMICONDUTOR USUAL



# NANOFITAS de GRAFENO



(c) Gap de transporte

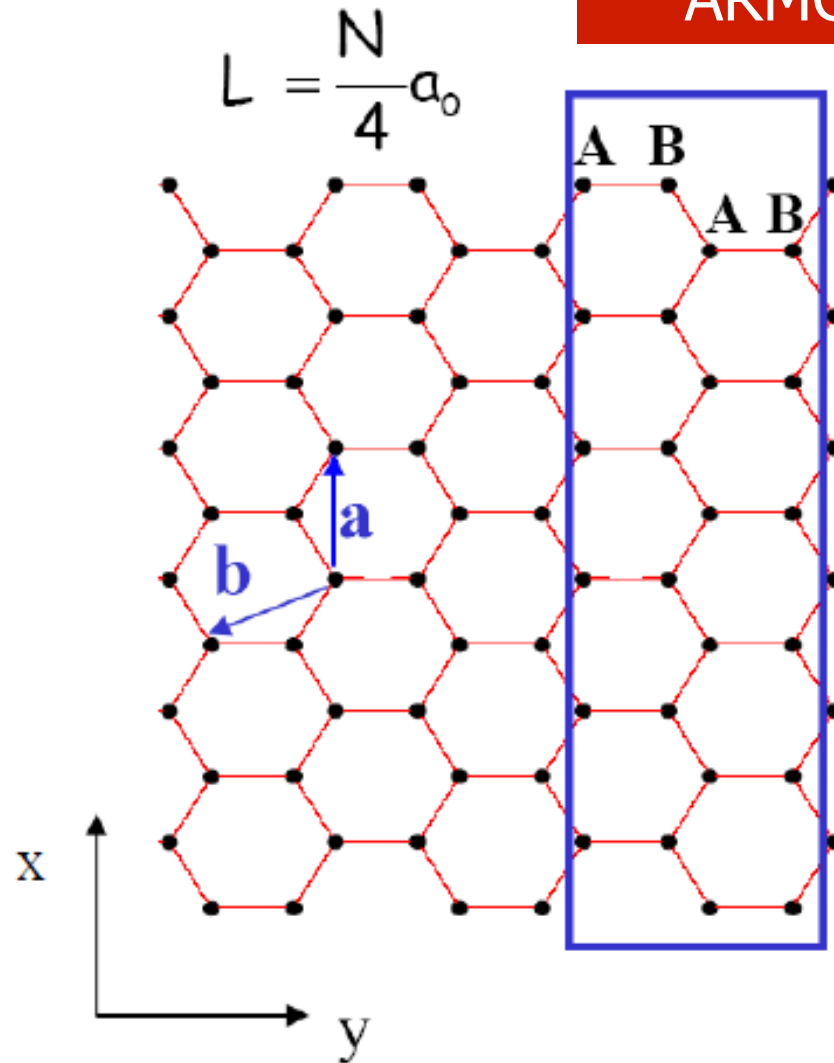
(d) Grande # de ressonâncias bem marcadas

C. Stampfer et al, PRL 102, 056403 (2009)

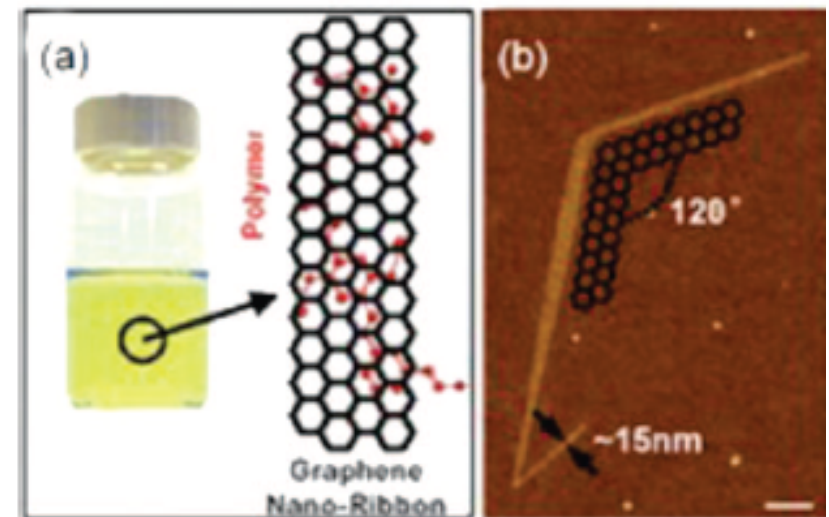




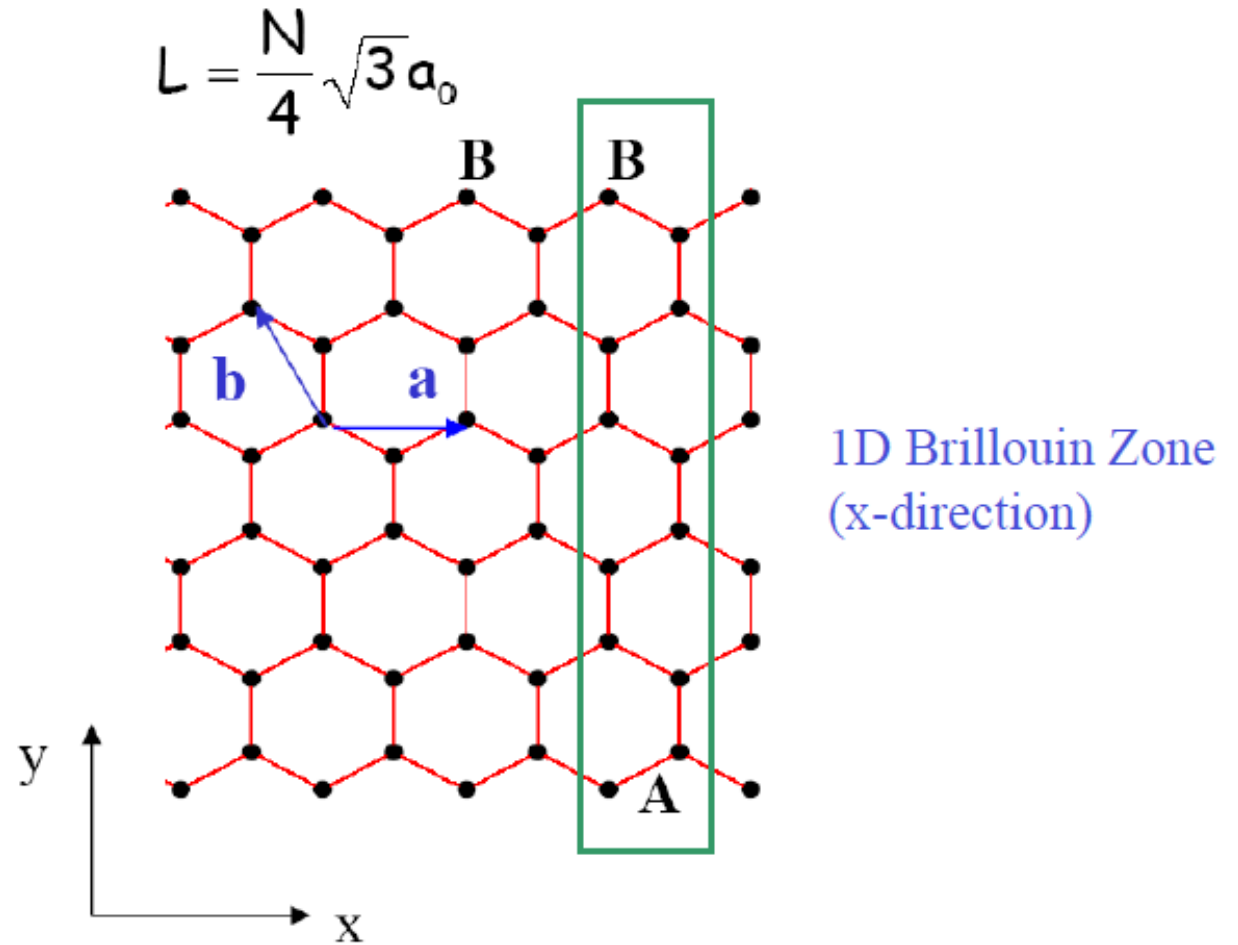
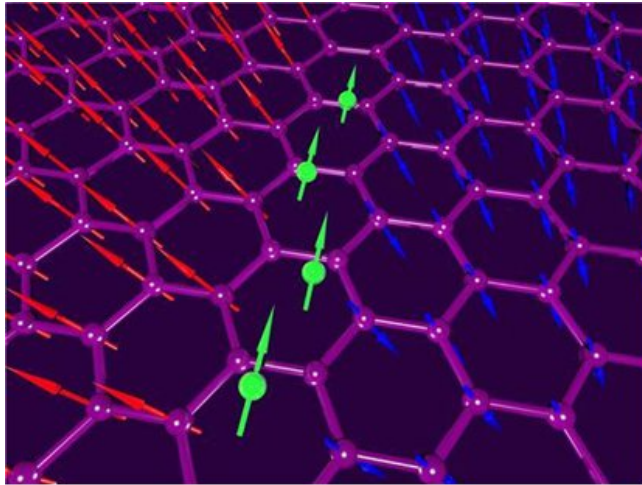
# ARMCHAIR GRAPHENE NANORIBBON



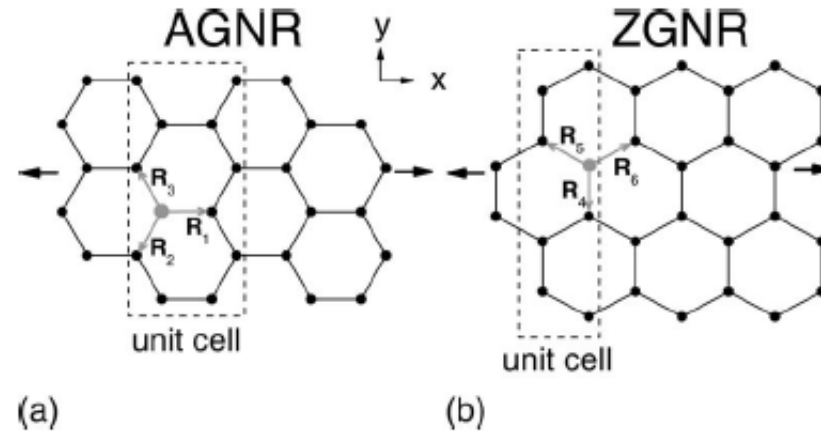
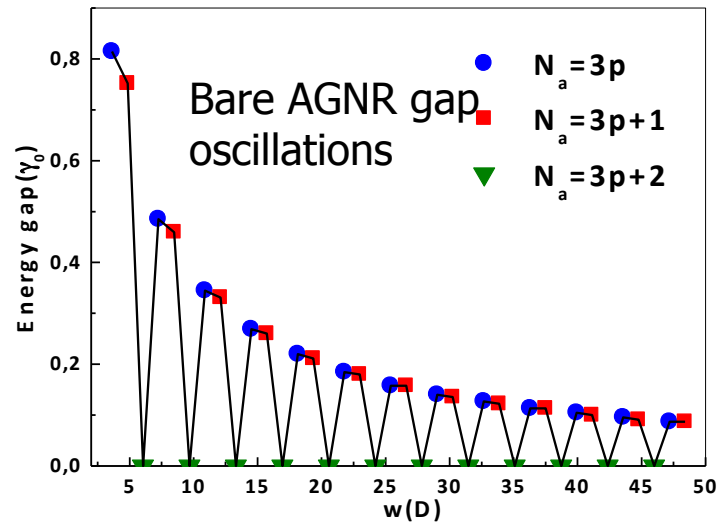
1D Brillouin Zone  
(x-direction)



# ZIGZAG GRAPHENE NANORIBBON



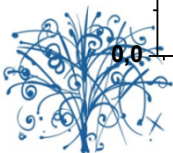
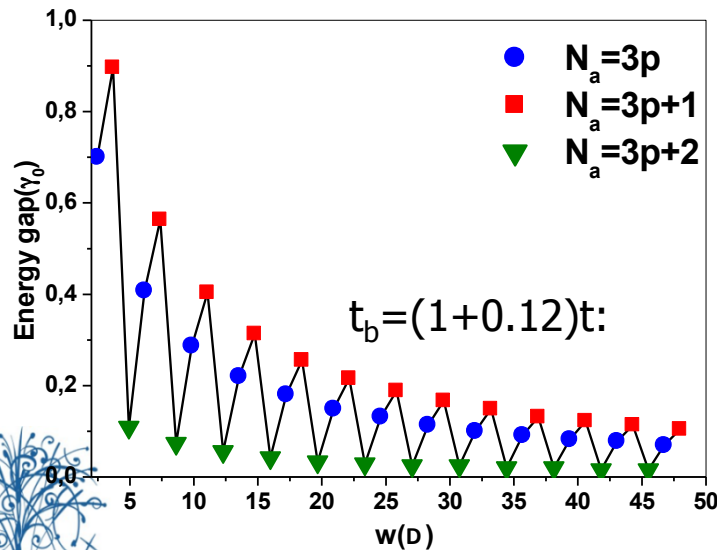
# MODELAGEM DO GAP DE ENERGIA DE NANOFITAS DE GRAFENO SOB A AÇÃO DE CAMPOS EXTERNOS



$$H = \sum_n^N \epsilon_n(E) c_n^\dagger c_n + \sum_{n,m}^N \gamma_{n,m}(B) c_n^\dagger c_m + h.c.,$$

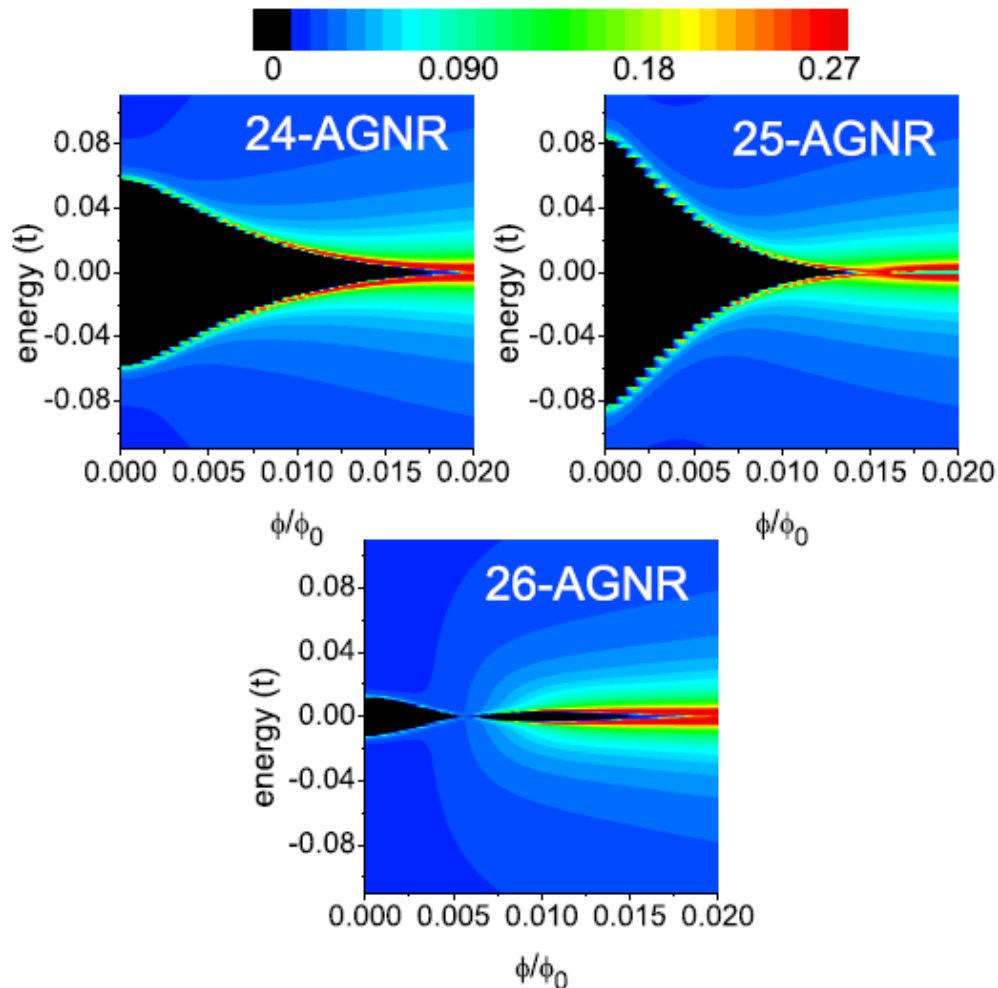
**CAMPO ELÉTRICO** – Potencial de Poison (auto-consistente)

**CAMPO MAGNÉTICO** – Peirls approx.

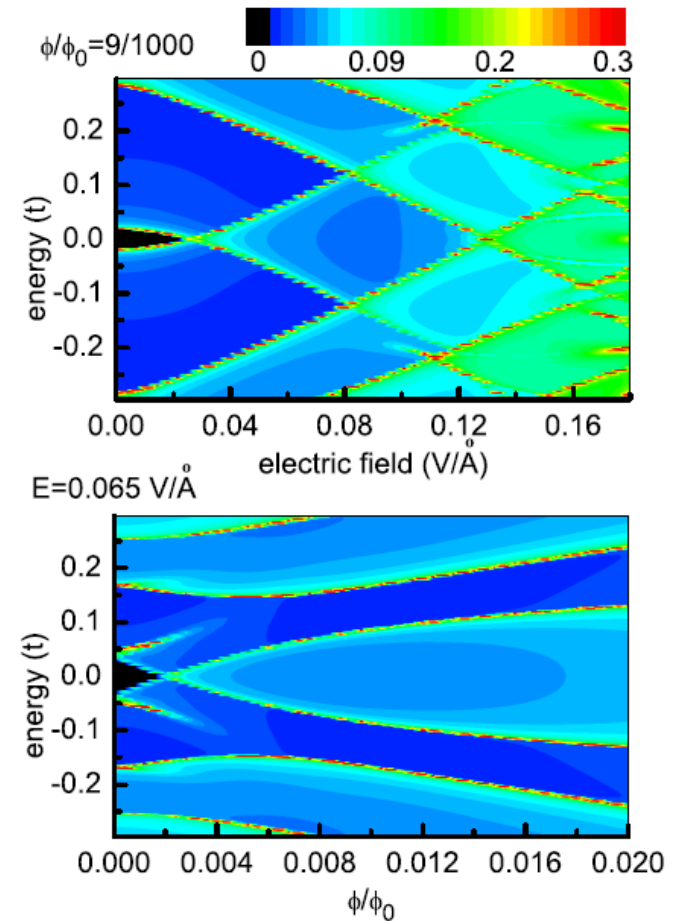


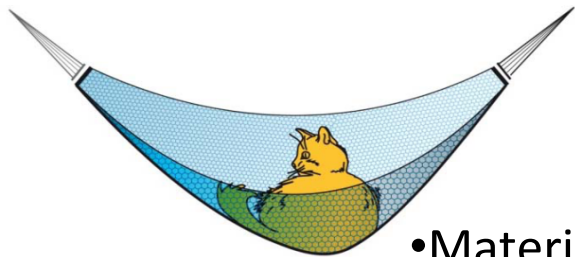


# ALTERANDO OS GAPS campos externos E & B



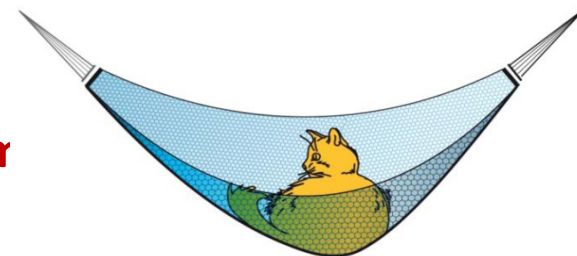
C. Ritter, S. Makler, A Latgé *Phys. Rev. B* 77, 195443 (2008)



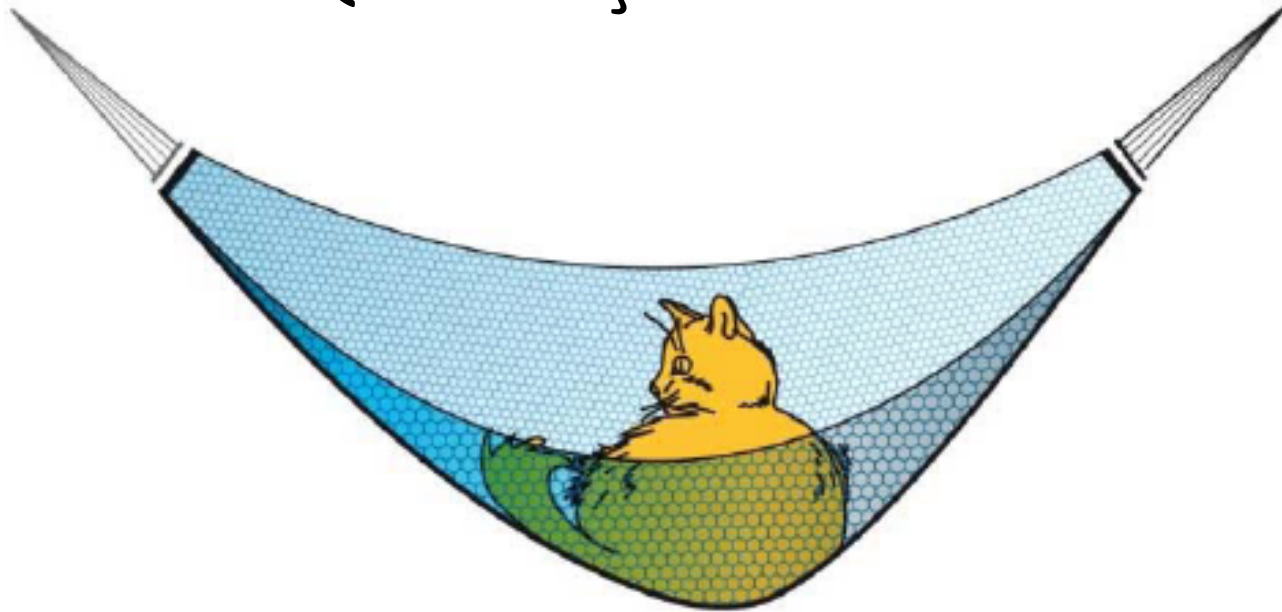


## POR QUE TANTO INTERESSE NO GRAFENO?

- Material mais forte já medido: Módulo de Young -  $1.0 \text{ TPa}$  ( $10^{12}$ )
- Membrana flexível mais fina jamais criada ( $0.35 \text{ nm}$ )
- Impermeável à gases (mesmo Hidrogênio atômico)
- Transporte Balístico sobre  $\mu\text{m}$  (temperatura ambiente)
- Valor Recorde de condutividade térmica à temperatura ambiente ( $\sim 5000 \text{ W/mK}$ )
- Densidade de corrente 6 ordens de magnitude maior do que para o Cu
- Quantum Hall Effects (temperatura ambiente)
- 2 átomos - área de  $0.052 \text{ nm}^2$  dens =  **$0.77 \text{ mg/n}$**



# GRAFENO É MAIS DO QUE 100 VEZES MAIS RESISTENTE DO QUE O AÇO MAIS FORTE



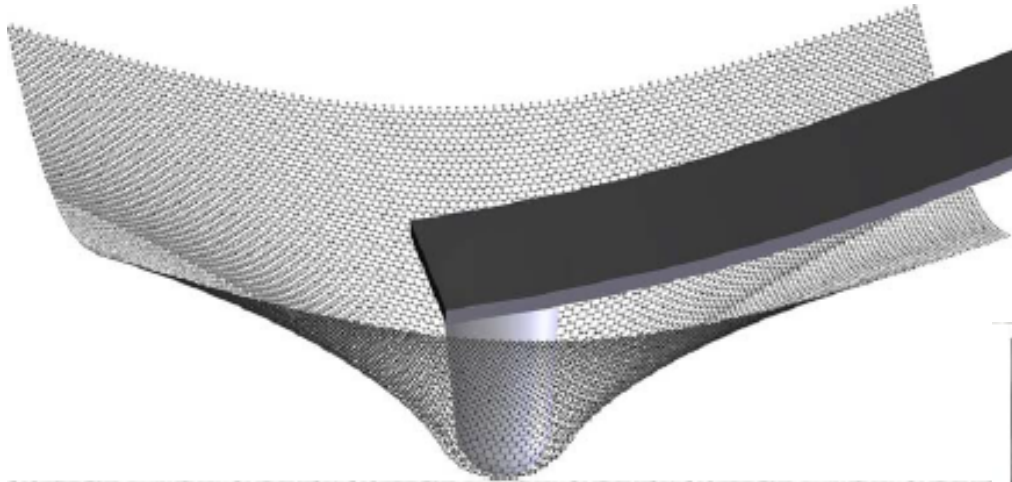
[Can put a 4Kg mass (e.g. a cat) on a 1 m<sup>2</sup> graphene (if one can make it).  
Cartoon taken from Nobel Prize announcement]





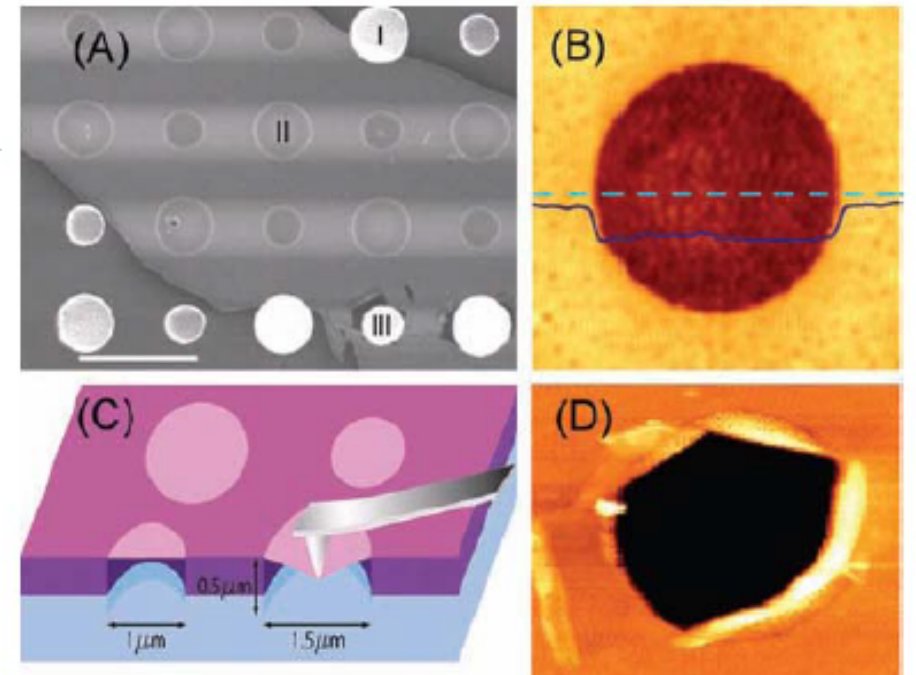
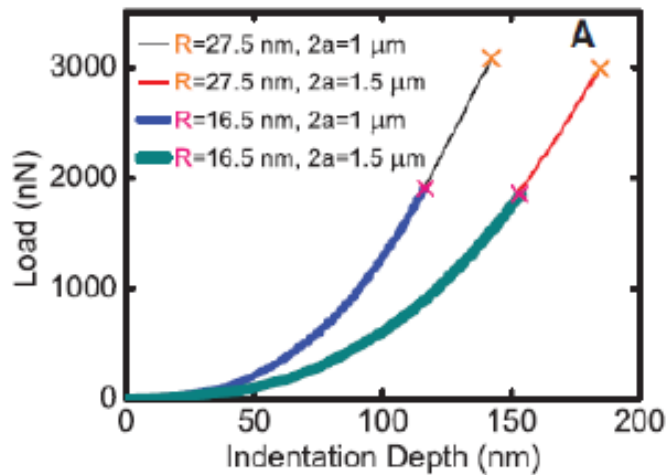
# PROPRIEDADES MECÂNICAS DO GRAFENO

## Forte e Resistente



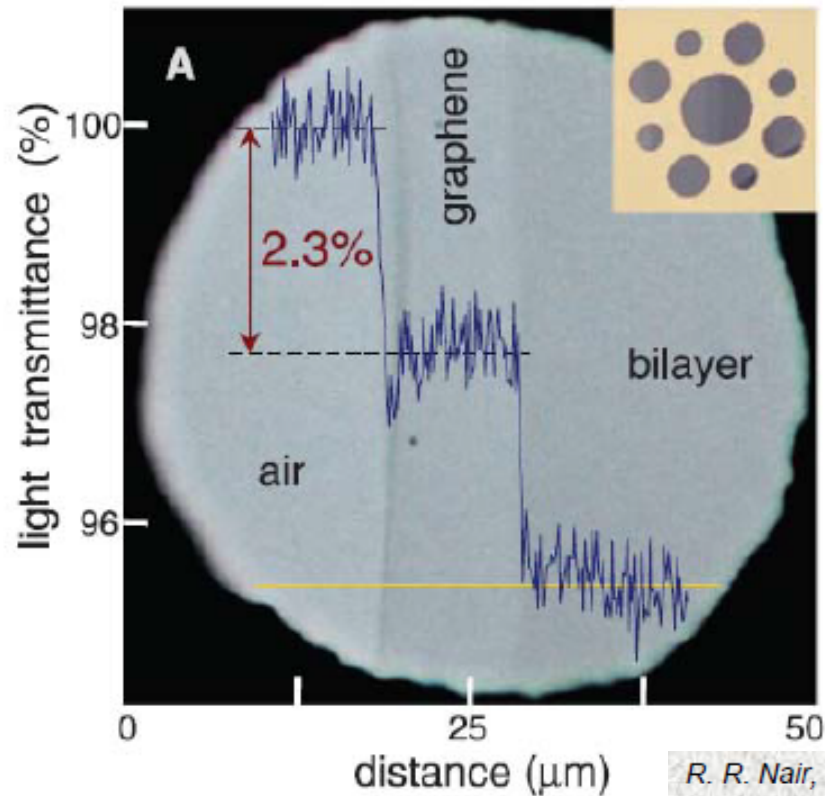
Young's modulus: 1 TPa (Steel ~ 0.2 TPa)

C. Lee, X. Wei, J. W. Kysar, & J. Hone, *Science* 321, 385 (2008)



## PROPRIEDADES ÓPTICAS: QUASE TRANSPARENTE

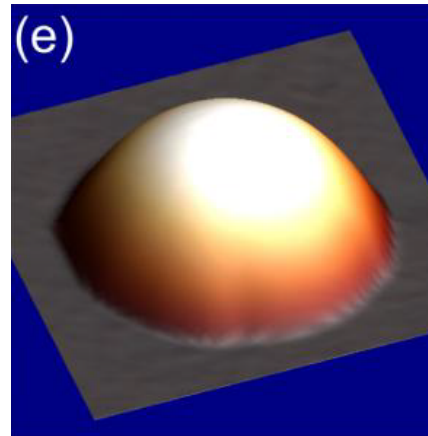
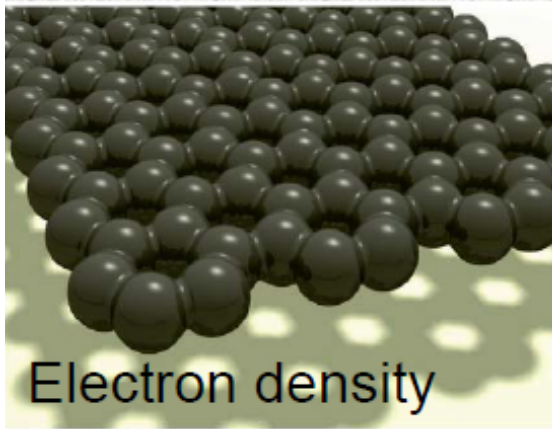
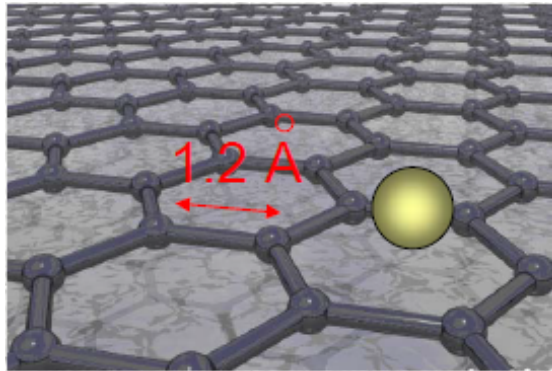
**MEMBRANA** de apenas 1 átomo de espessura  
- útil para dispositivos



*R. R. Nair, P. Blake, A. N. Grigorenko, K. S. Novoselov, T. J. Booth, T. Stauber, N. M. R. Peres, & A. K. Geim  
Science **320**, 1308 (2008).*



# MEMBRANAS IMPERMEÁVEIS

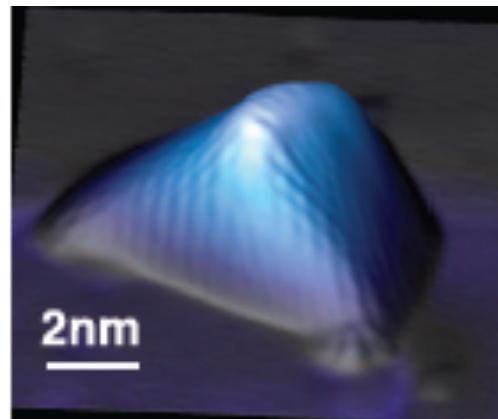


T. Georgiou et al

APPLIED PHYSICS LETTERS 99, 093103 (2011)

## Graphene bubbles with controllable curvature

T. Georgiou,<sup>1</sup> L. Britnell,<sup>1</sup> P. Blake,<sup>2</sup> R. V. Gorbachev,<sup>2</sup> A. Gholinia,<sup>3</sup> A. K. Geim,<sup>2</sup> C. Casiraghi,<sup>4,5</sup> and K. S. Novoselov<sup>1,a)</sup>



## Strain-Induced Pseudo-Magnetic Fields Greater Than 300 Tesla in Graphene Nanobubbles

N. Levy,<sup>1,2,\*</sup> S. A. Burke,<sup>1,3,†</sup> K. L. Meaker,<sup>1</sup> M. Panlasigui,<sup>1</sup> A. Zetti,<sup>1,2</sup> F. Guinea,<sup>3</sup> A. H. Castro Neto,<sup>4</sup> M. F. Crommie<sup>1,2,§</sup>

30 JULY 2010 VOL 329 SCIENCE

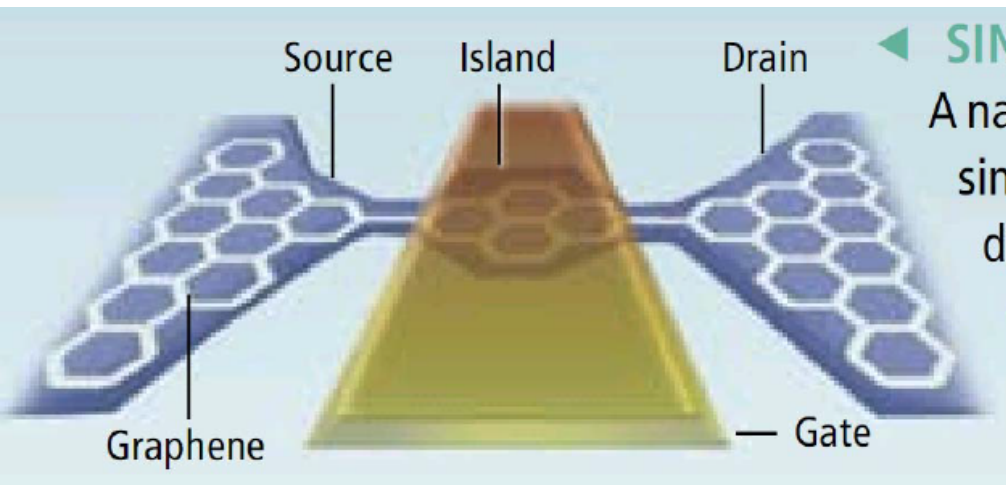




# GRAFENO – semicondutores excelentes

Eletrons se movem sem muita resistência no plano

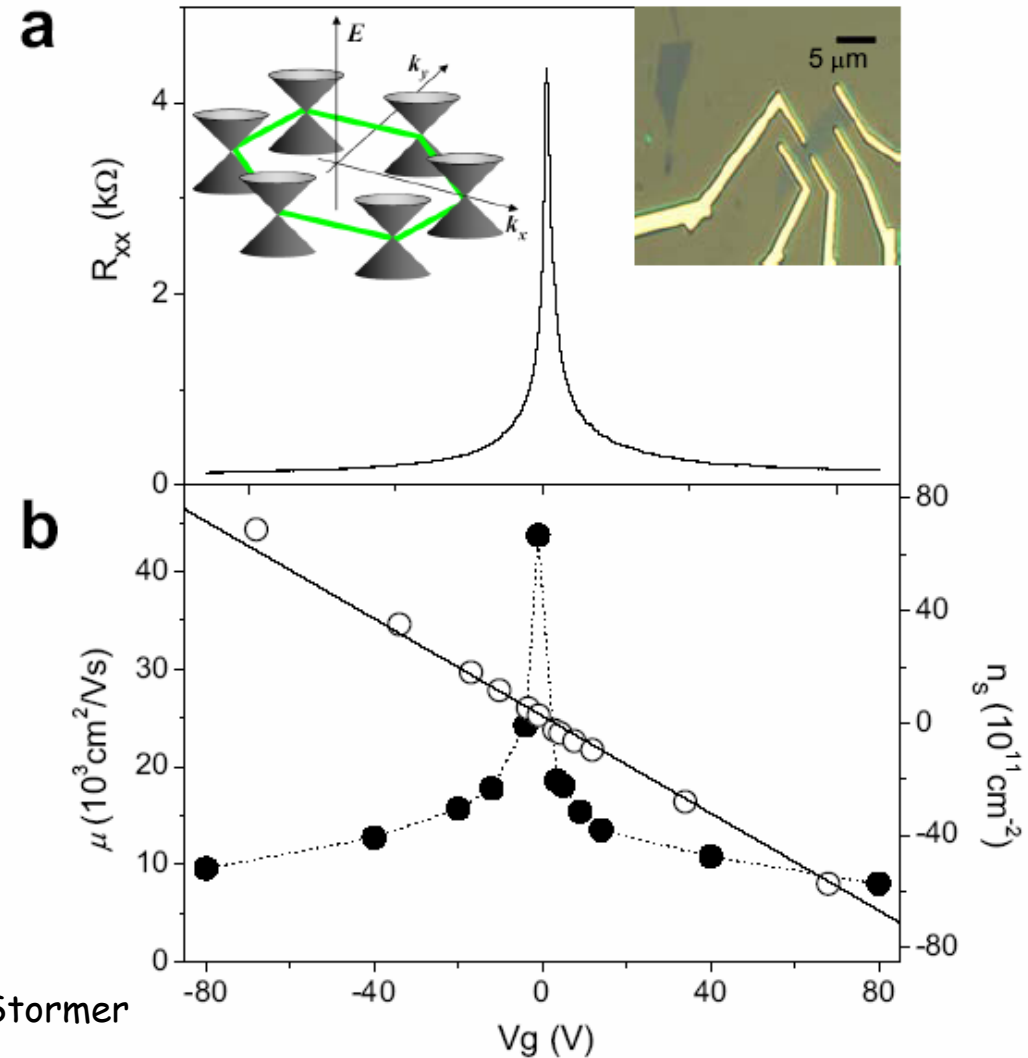
## TRANSITOR BASEADO EM GRAFENO



Scientific American, 2008 April, P.96



Yuanbo Zhang, Yan-Wen Tan, Horst L. Stormer  
& Philip Kim



Andrea Latgé 18/08/2015

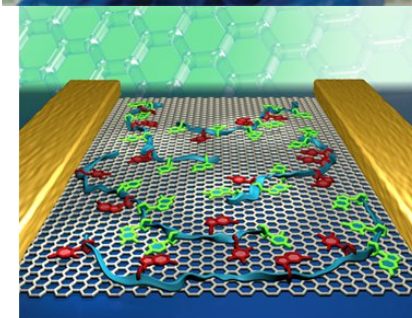
## 7. Future Work

Graphene has an interesting history, but many now wonder about its future. The subject of considerable scholarly debate, it does seem reasonable to assert a few things looking ahead. First, the quality and availability of “synthetic” graphene will continue to improve. Whether high quality material comes in the form of an alternative chemical route to the complete exfoliation of graphite or from optimization of the thermal processes required for substrate-based methods, there is no sign that synthetic techniques are nearing their upper limit. This means that device engineers will have ample access to improved materials for developing novel structures and finding ways to integrate graphene into present-day electronic devices.

*Chem. Rev.* 2010, 110, 132–145

### Honeycomb Carbon: A Review of Graphene

Matthew J. Allen,<sup>†</sup> Vincent C. Tung,<sup>‡</sup> and Richard B. Kaner<sup>\*,†,‡</sup>



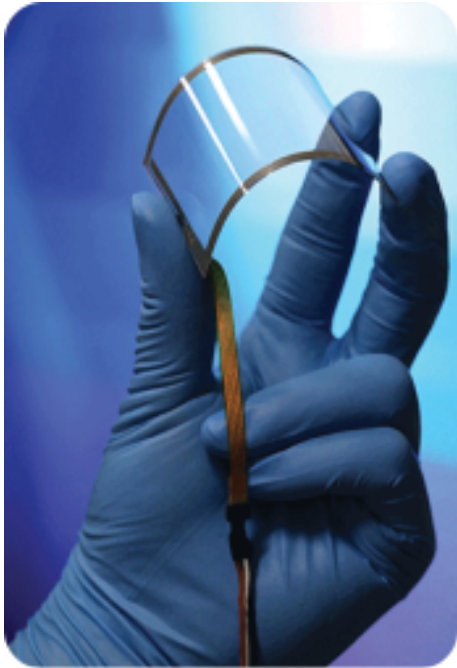
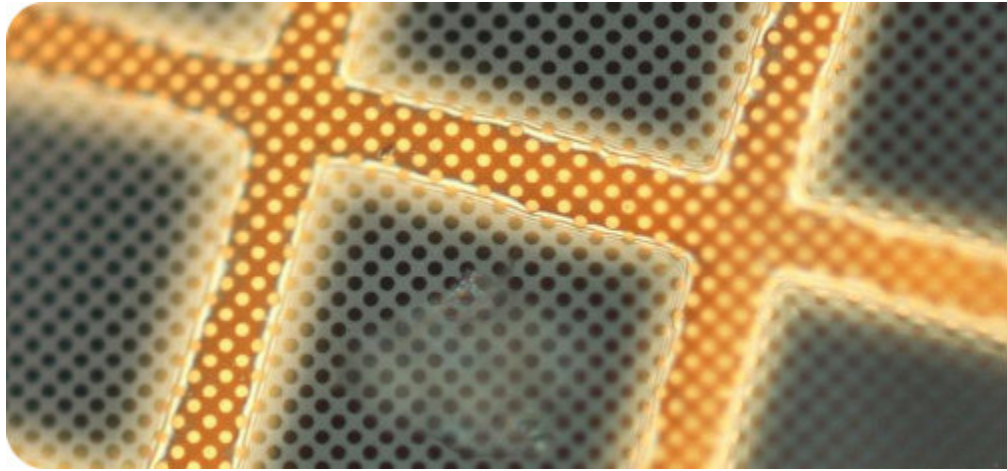
Second, chemical modification of graphene's basal plane or its edges will substantially influence graphene-based devices. For electronic applications, one can imagine the attachment of functional groups aimed at self-assembly of simple circuits or the incorporation of chemical dopants to limit leakage current under zero gate bias. For sensors, lock-and-key type binding sites could provide selective sensitivity to a wide variety of analytes. These might include chemical warfare agents or even biological species.

Third, industrial use of graphene as a transparent conductor could have huge implications for the solar industry. As synthetic routes improve, the prospect of replacing ITO with a low-cost carbon-based coating seems feasible. This would not only remove significant uncertainty about the availability and cost of indium but also enable nonevaporative roll-to-roll processing of transparent conductors.





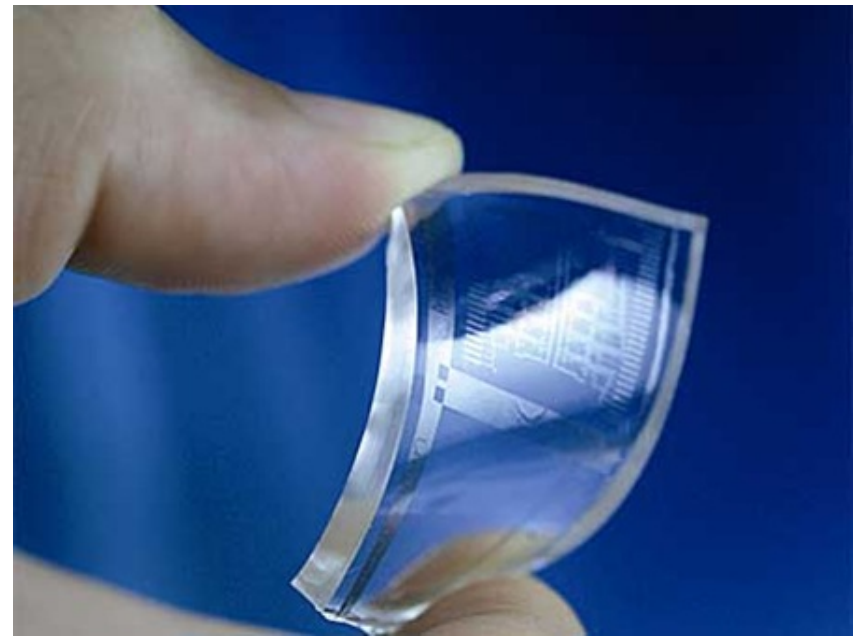
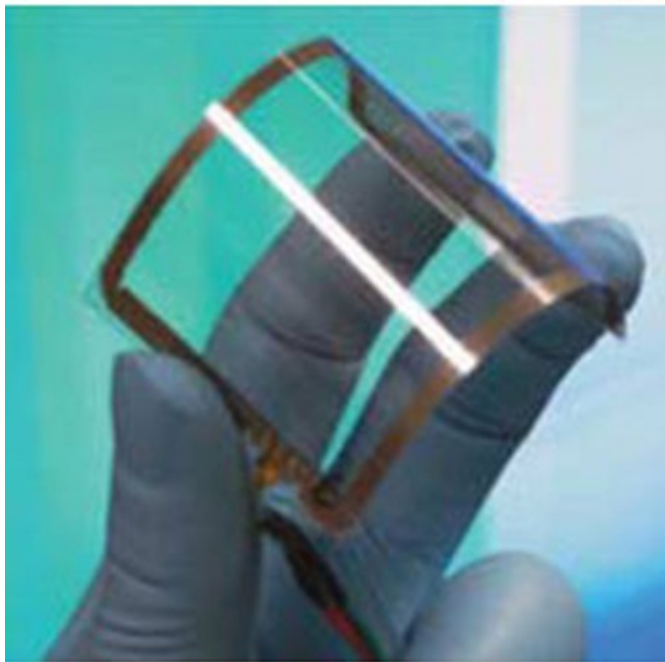
**Graphene tem propriedades extraordinárias que devem levar a grandes revoluções de muitas áreas tecnológicas**



As propriedades do grafeno os torna atrativ ara aplicações em eletrônica flexível. Eles tb usam empilhamneto camada por camada para fabricar um filme de 4 camadas dopadas com propriedades superiores `as de electodos transparentes comerciais como os óxidos de índio. A fotografia sobre a capa mostra um dispositivo "flexible touch-screen" contendo eletrodos de graphene.

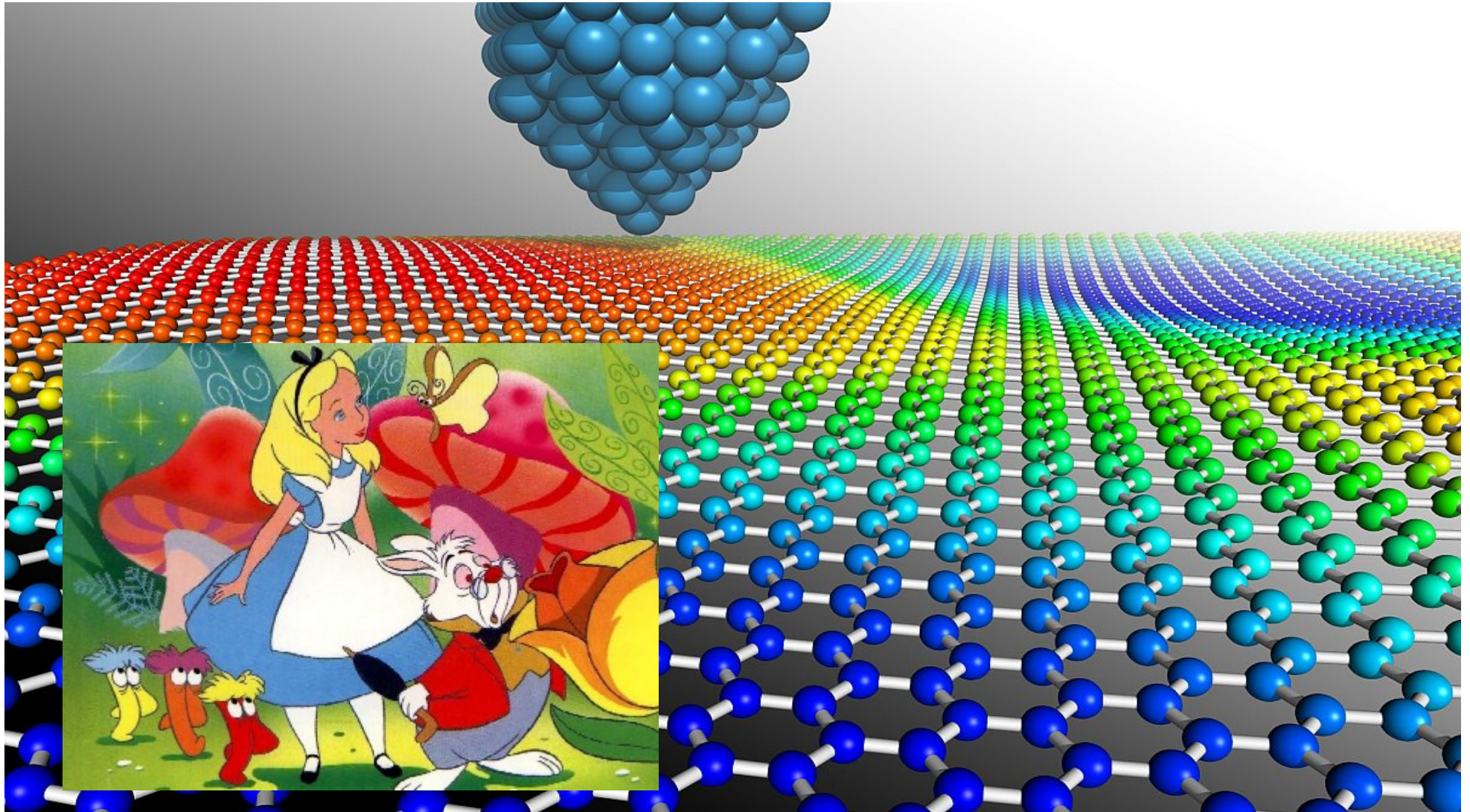
Contact: [Prof. Kostya Novoselov](#), [Dr. Peter Blake](#)







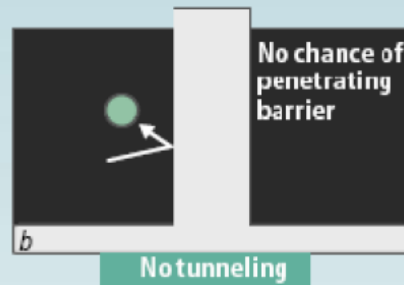
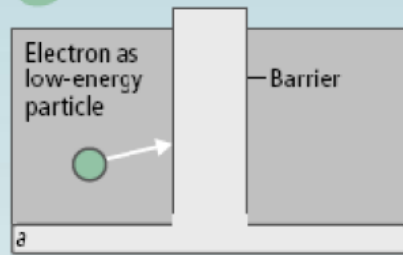
# VENHAM CONHECER MAIS DE PERTO O MUNDO MARAVILHOSO DO CARBONO



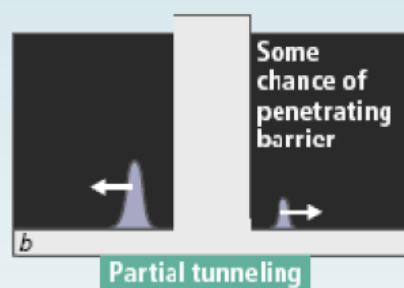
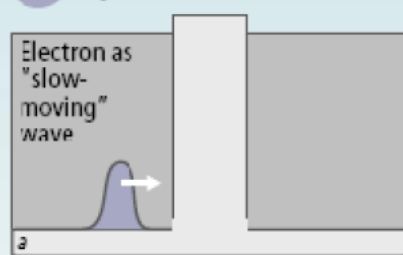




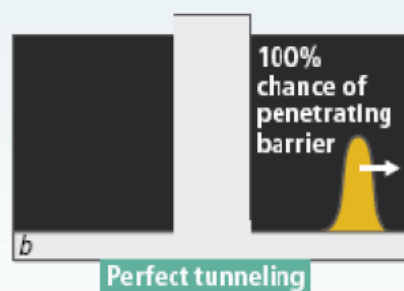
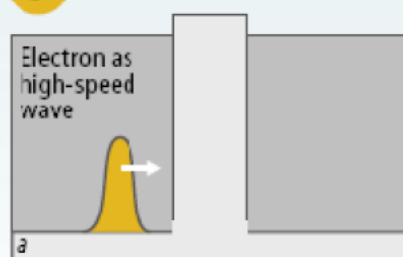
### 1 CLASSICAL PHYSICS



### 2 QUANTUM MECHANICS



### 3 QUANTUM ELECTRODYNAMICS



Klein paradox: **transmission of relativistic particles is unimpeded even by highest barriers**

The transmission probability  $T$  depends only weakly on the barrier height, approaching the **perfect transparency** for very high barrier

A. K. Geim & P. Kim Scientific American, Apr. 2008





# A escala "NANO"

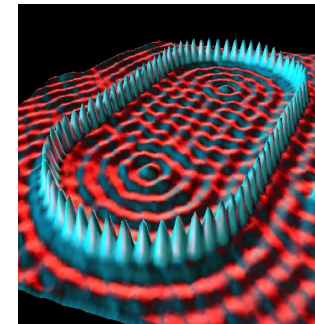
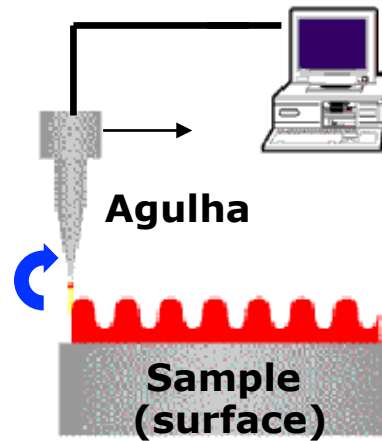
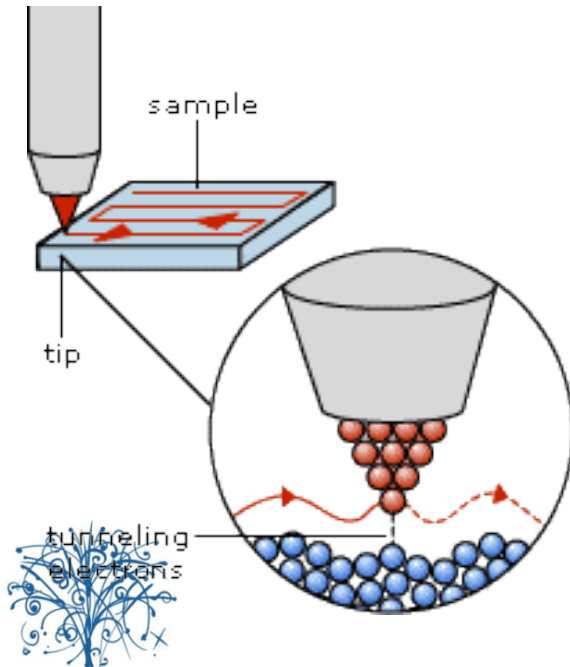
**"Nanotechnology" foi mencionado pela primeira vez em 1959 pelo físico *Richard Feynman***

"What I want to talk is about the problem of manipulating things in atomic scales".

"Why we can not write the full 24 volumes of the British Encyclopedic in the small pin?"

**Richard P. Feynman Nobel Price Physics-1965**

## Como ver o átomo ?



**Scanning Tunneling  
Microscope - STM**

Blue Platinum  
The surface of Platinum.

