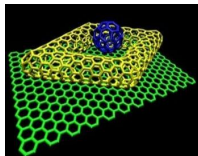


A 3D molecular model of a nanomaterial. It features a large, flat, green hexagonal lattice representing a graphene sheet. On top of this sheet is a smaller, yellow, cage-like structure, possibly a carbon nanotube or a similar nanoscale framework. A blue, spherical molecule with a complex internal structure is positioned on top of the yellow structure. The entire model is set against a black background.

Física Computacional e o Estudo de Nanomateriais

Eduardo Costa Girão

Universidade Federal do Piauí



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Sigam @nanofisica no Instagram.

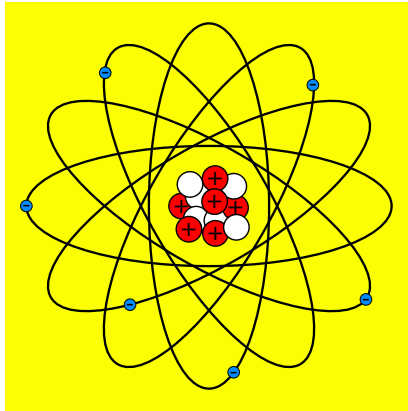
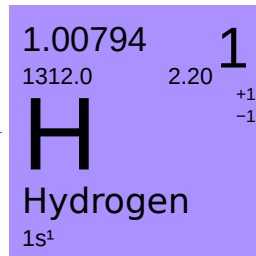
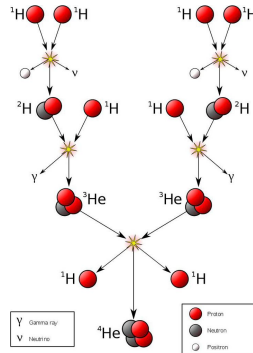


Tabela Periódica

Periodic Table of The Elements

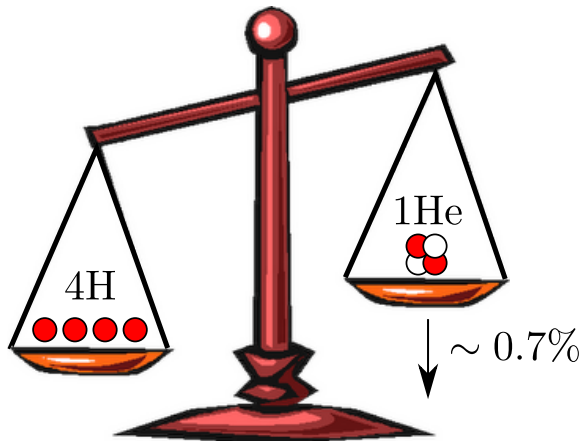
The periodic table shows elements arranged by atomic number (1 to 118). Hydrogen (H) is located at the top-left, with atomic number 1. A red circle highlights it, and a red arrow points from it to a larger, detailed view of Hydrogen on the right.

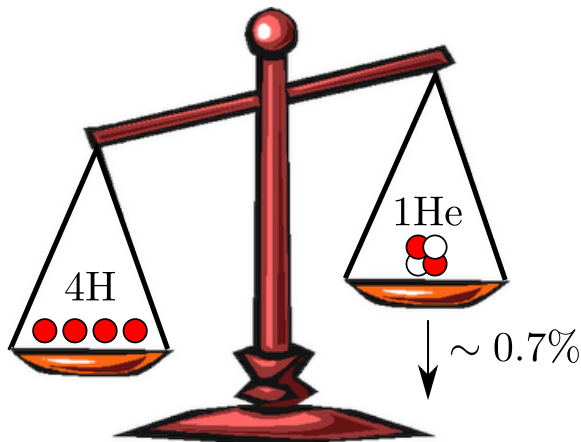




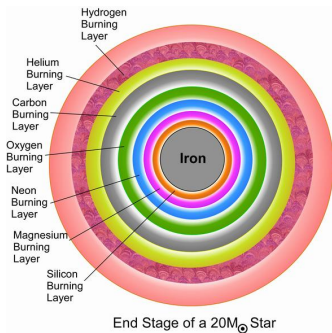
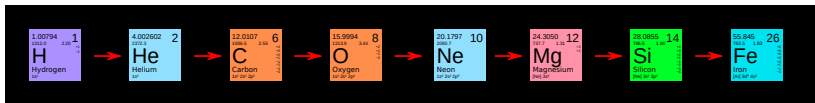
“The Sun’s Energy Doesn’t Come From Fusing Hydrogen Into Helium (Mostly)”, Forbes.

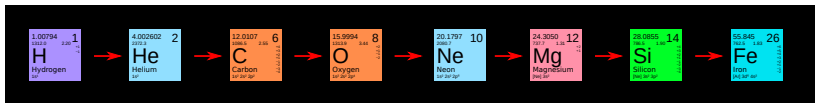
<https://www.forbes.com/sites/startswithabang/2017/09/05/the-suns-energy-doesnt-come-from-fusing-hydrogen-into-helium-mostly/?sh=765df6f970f9>



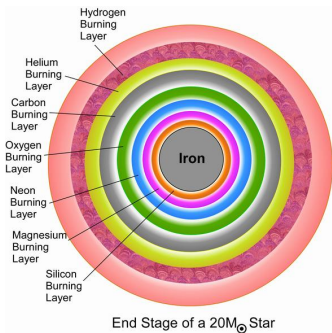


$$E = mc^2$$

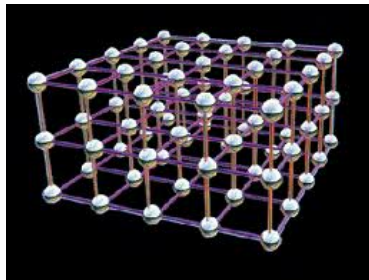
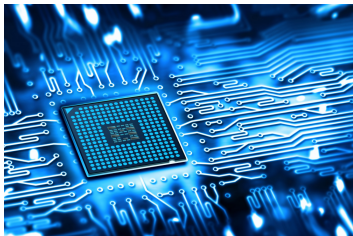
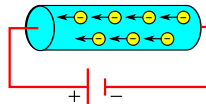


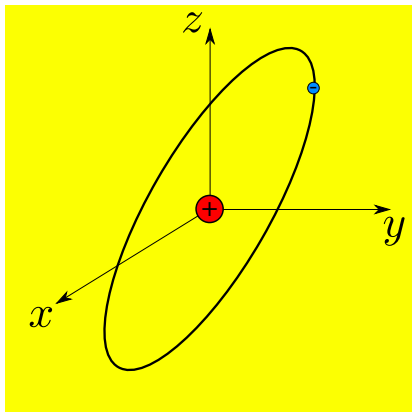


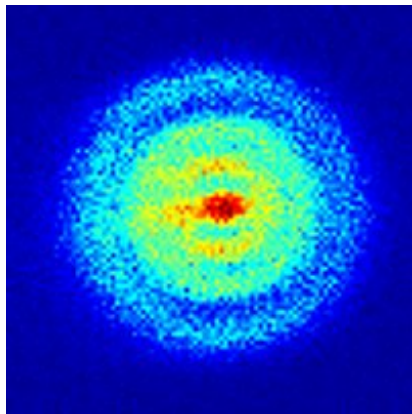
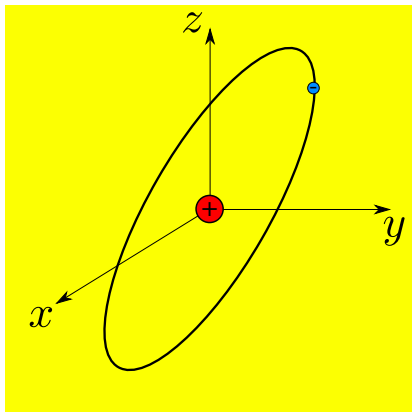
Supernova



Moldando e Manipulando a Matéria

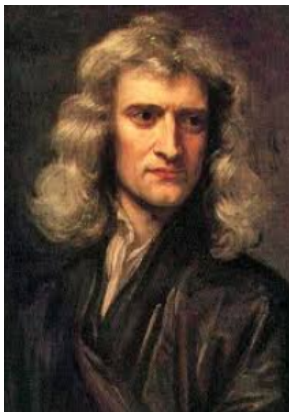






PRL **110**, 213001 (2013).

Objetos macroscópicos:



Leis de Newton

$$\vec{F} = m\vec{a}$$



Objetos microscópicos:



Princípio de Incerteza de Heisenberg

$$\Delta x \cdot \Delta p \geq \frac{\hbar}{2}$$

$$\hbar = \frac{h}{2\pi}$$

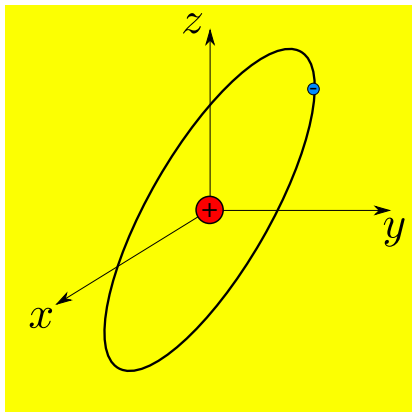
Objetos microscópicos:



Equação de Schrodinger

$$\hat{H}\psi = E\psi$$

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}(x)$$



- $n = 1, 2, 3, \dots$
- $l = 0, 1, 2, \dots, n - 1$
- $m = -l, -(l - 1), \dots, l - 1, l$

$$\hat{H} = \frac{-\hbar^2}{2m} \nabla^2 + V(r)$$

Relações de Comutação

$$[\hat{H}, \hat{L}^2] = 0 \quad [\hat{H}, \hat{L}_z] = 0 \quad [\hat{L}^2, \hat{L}_z] = 0.$$

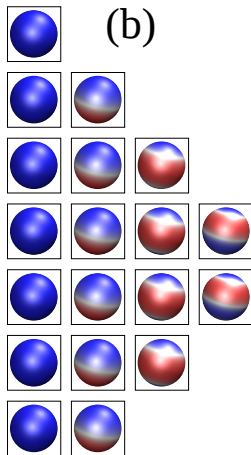
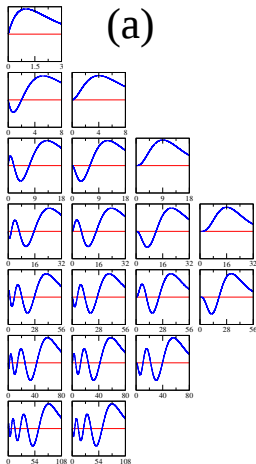
Autofunções de Onda

$$\psi_{n,l,m}(r, \theta, \varphi) \sim r^l e^{-\alpha r} L_{n-l-1}^{2l+1}(2\alpha r) Y_{l,m}(\theta, \varphi)$$

Autovalores de Energia

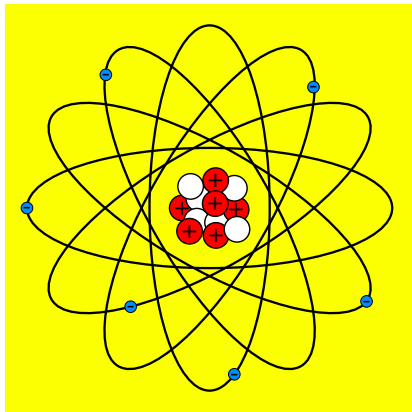
$$E_n = -\frac{\hbar^2 Z^2}{2ma_0^2 n^2} = -\frac{mZ^2 e^4}{32\pi^2 \epsilon_0^2 \hbar^2 n^2}$$

Orbitais Atômicos



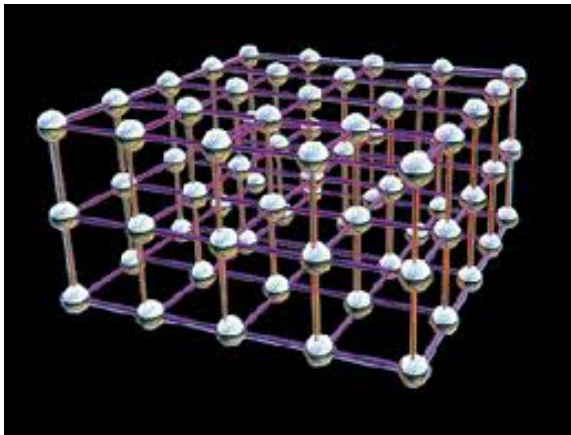
(c)

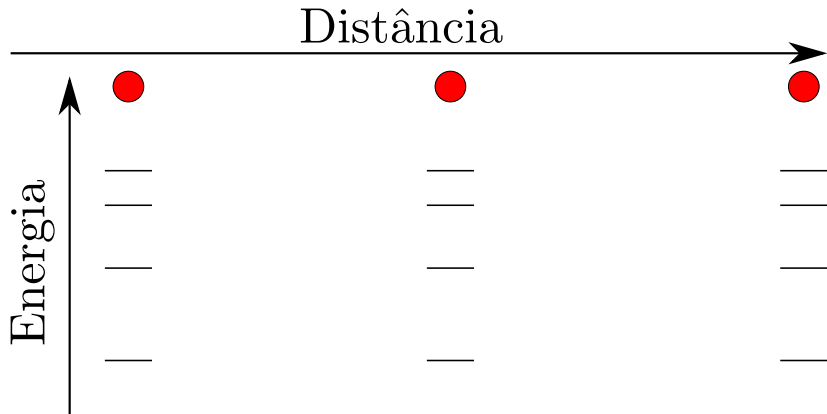
1s			
2s	2p		
3s	3p	3d	
4s	4p	4d	4f
5s	5p	5d	5f
6s	6p	6d	
7s	7p		

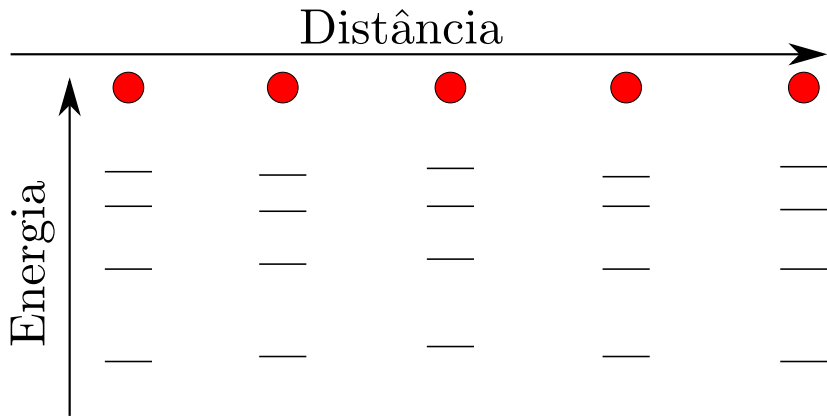


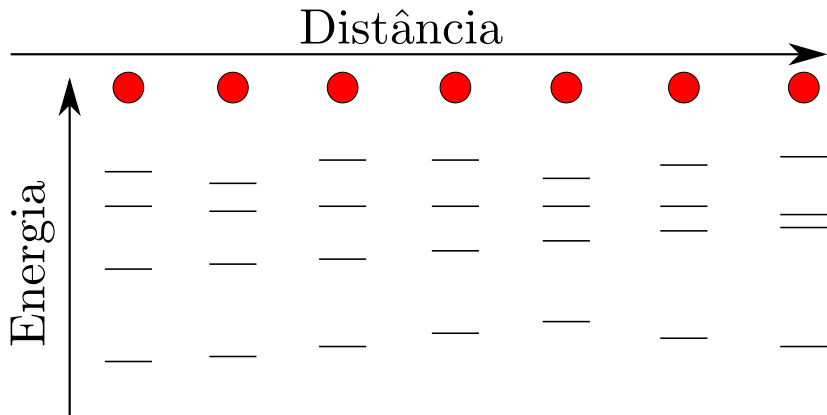
$$\hat{H}\psi = E\psi$$

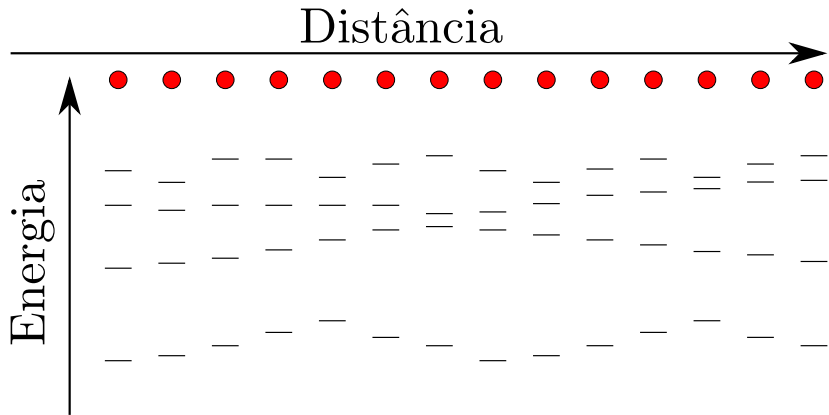
- Interação eletrônica correlaciona os movimentos dos elétrons;
- Solução analítica impossível;
- Métodos computacionais aproximados;
- O conceito de orbital ainda é útil de forma aproximada.

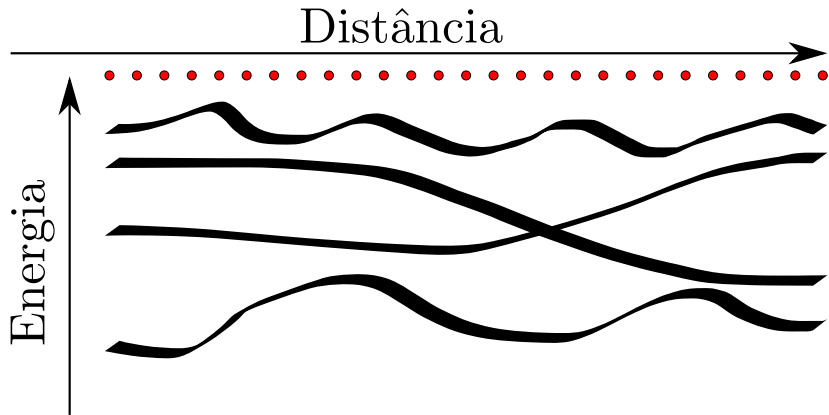


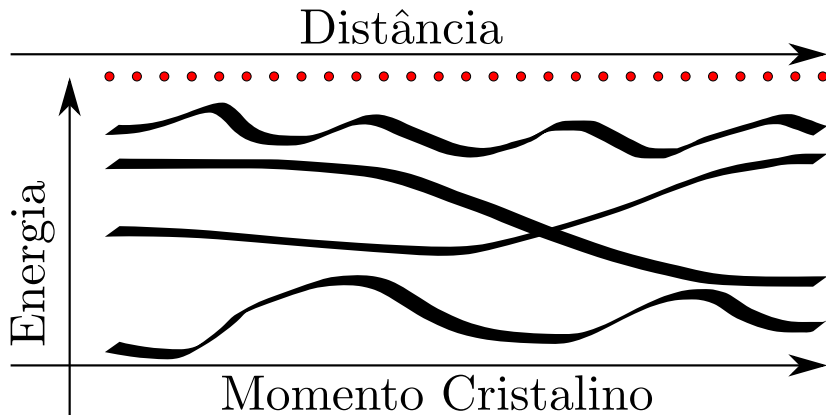


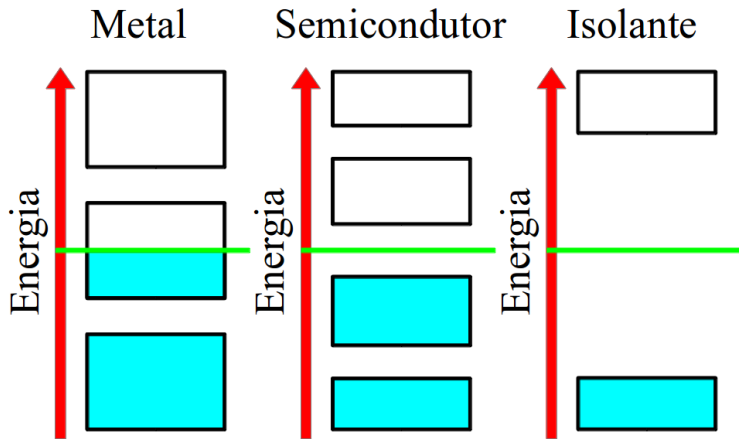


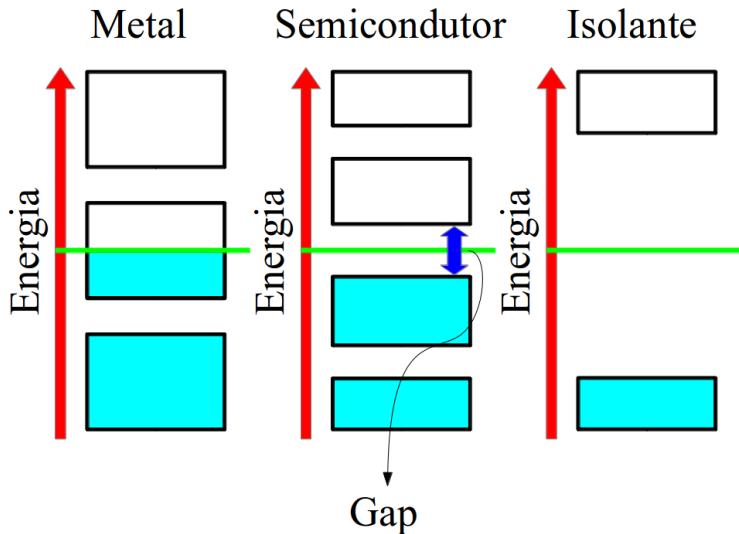






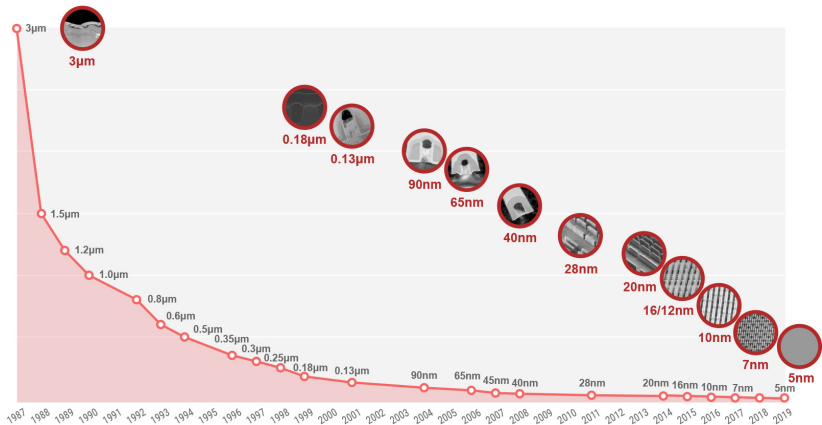






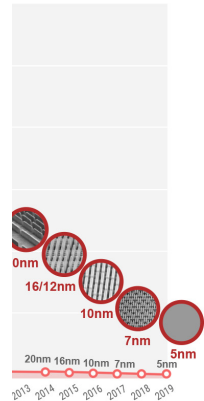
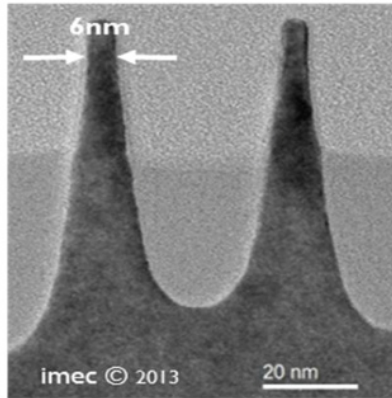
Miniaturização

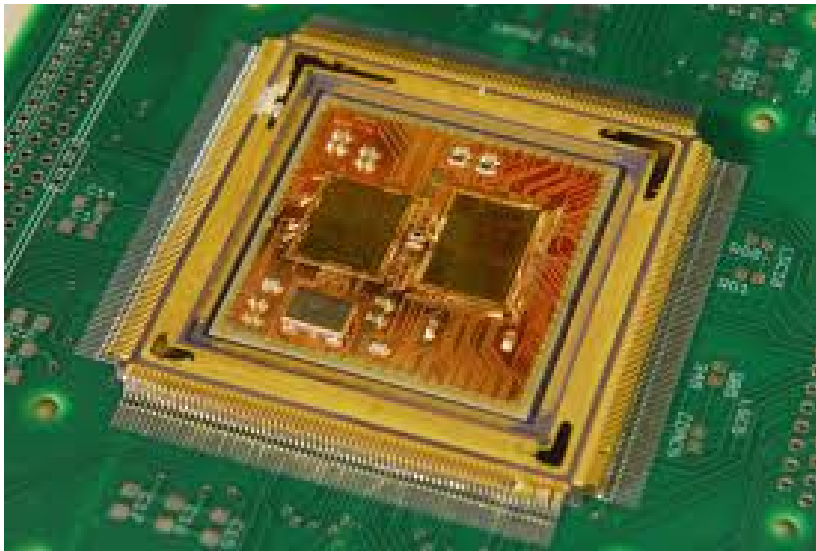
https://www.tsmc.com/english/dedicatedFoundry/technology/logic/l_5nm



Miniaturização

https://www.tsmc.com/english/dedicatedFoundry/technology/logic/l_5nm







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Rep. Prog. Phys. **68** (2005) 2701–2746

[doi:10.1088/0034-4885/68/12/R01](https://doi.org/10.1088/0034-4885/68/12/R01)

Physical limits of silicon transistors and circuits

Robert W Keyes

IBM Research Division, Yorktown, NY 10598, USA

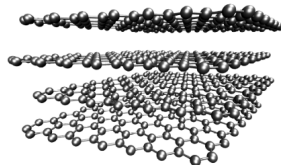
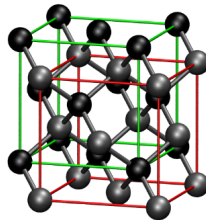
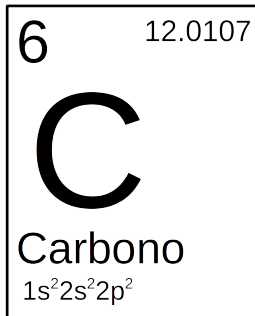
Received 27 April 2005, in final form 11 August 2005

Published 19 September 2005

Online at stacks.iop.org/RoPP/68/2701



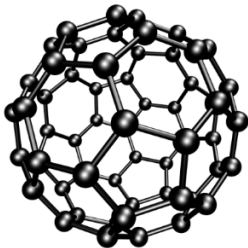
O caso do Carbono



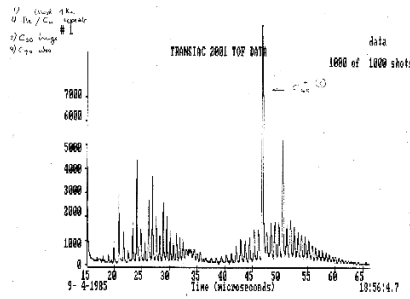
O caso dos Nanocarbonos



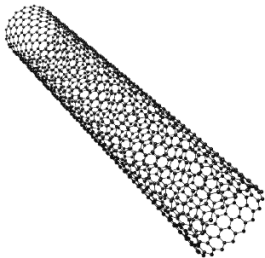
1985



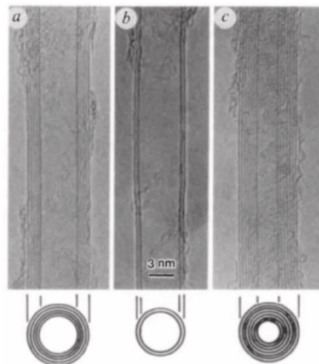
Nature **318**, 162 (1985).



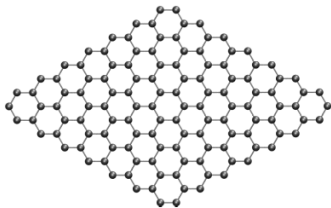
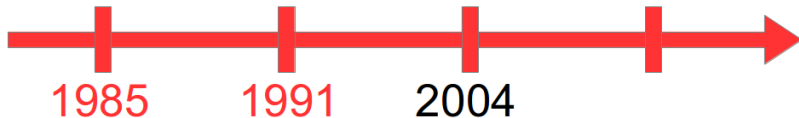
O caso dos Nanocarbonos



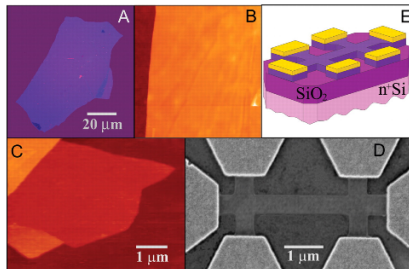
Nature **354**, 56 (1991).



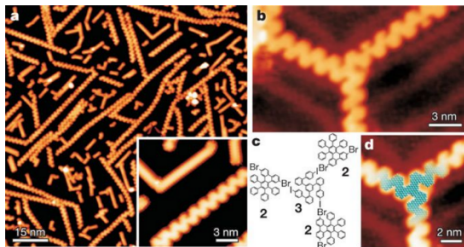
O caso dos Nanocarbonos



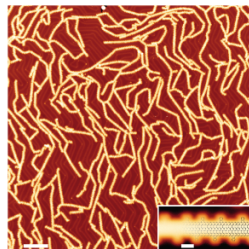
Science **306**, 666 (2004).



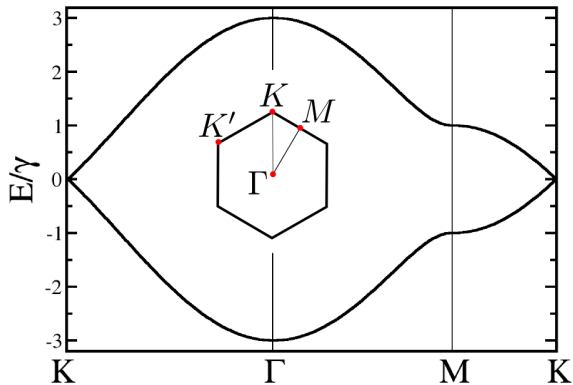
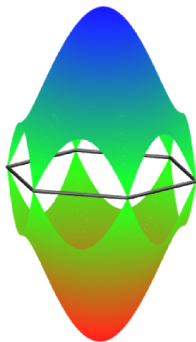
O caso dos Nanocarbonos



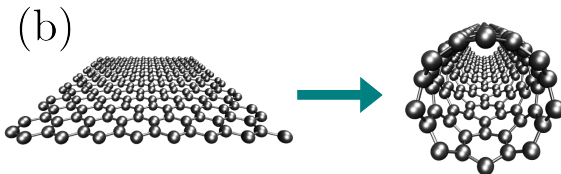
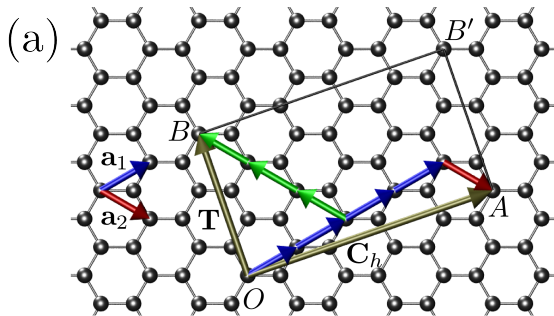
Nature **466**, 470 (2010).



Nature **531**, 489 (2016).

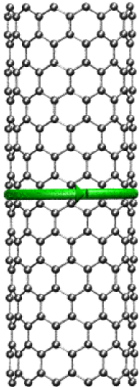


Nanotubos de Carbono

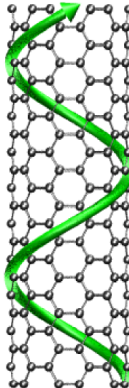


Nanotubos de Carbono

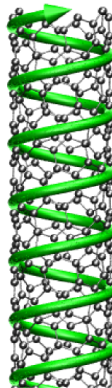
$(12,0)$



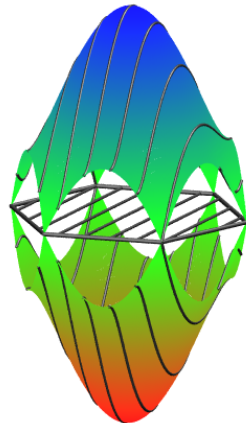
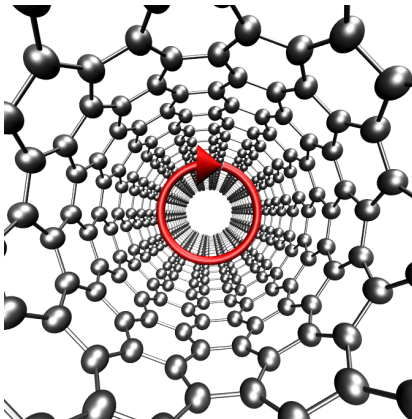
$(6,6)$



$(8,2)$



Nanotubos de Carbono

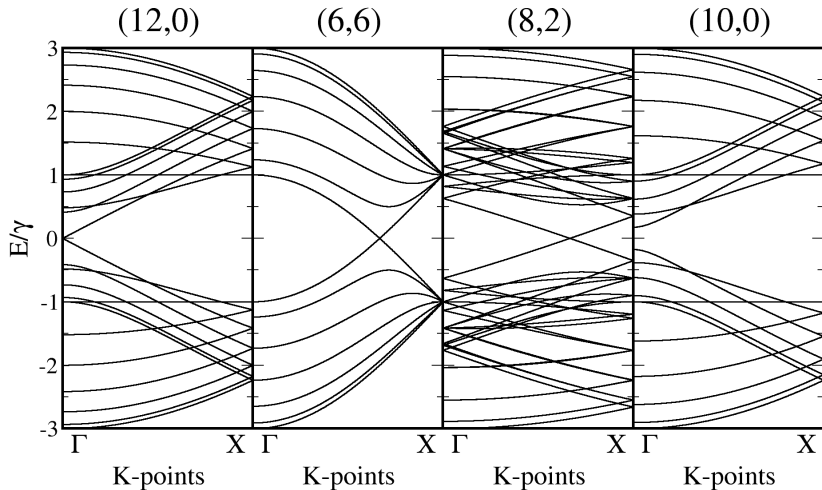


Metal 1 (M1): $\text{mod}(n - m, 3) = 0$; $\text{mod}(n - m, 3d) \neq 0$

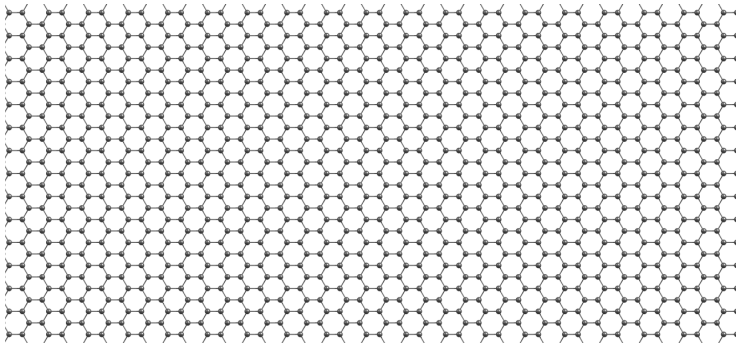
Metal 2 (M2): $\text{mod}(n - m, 3) = 0$; $\text{mod}(n - m, 3d) = 0$

Semiconducting (S): $\text{mod}(n - m, 3) \neq 0$; $d = \text{gcd}(n, m)$

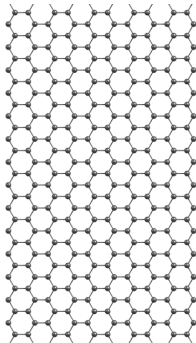
Nanotubos de Carbono



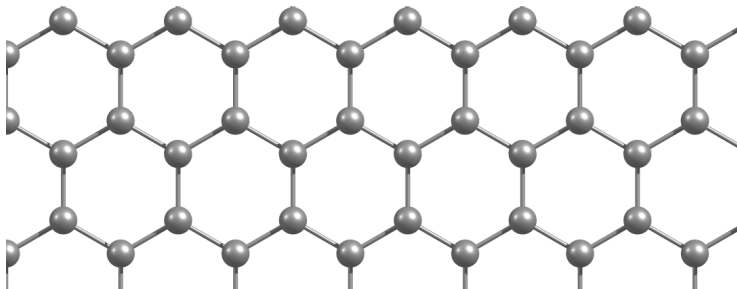
Nanofitas de Grafeno



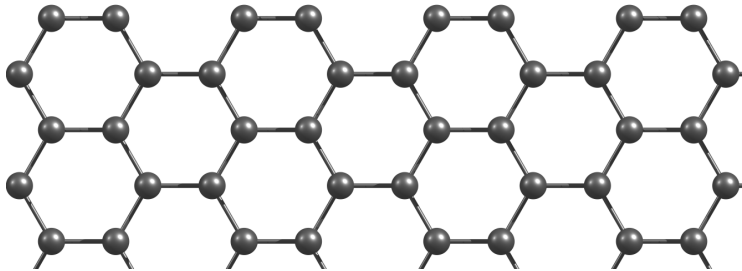
Nanofitas de Grafeno



Nanofitas de Grafeno - Caso Zigzag

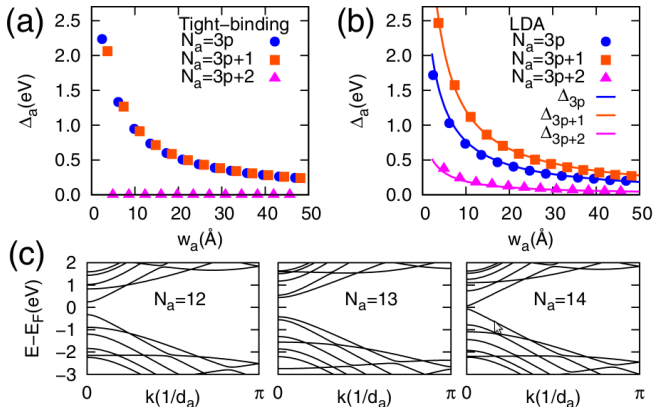


Nanofitas de Grafeno - Caso Armchair



Nanofitas de Grafeno - Caso Armchair

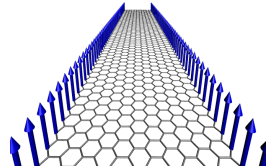
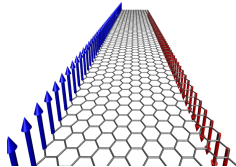
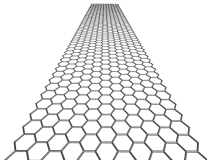
- A-GNRs são semicondutoras.



Y. S. son et al., Phys. Rev. Lett. **97**, 216803 (2006).

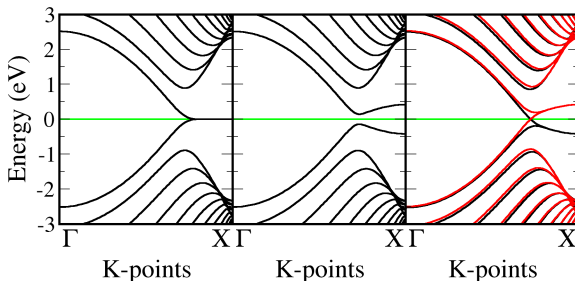
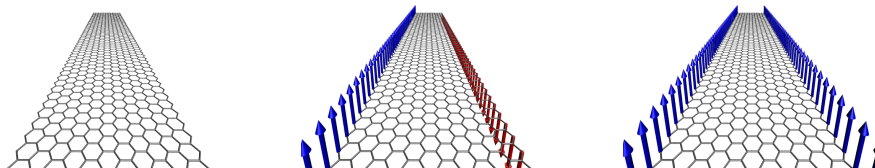
Nanofitas de Grafeno - Caso Zigzag

- Z-GNRs possuem um conjunto de estados magnéticos.



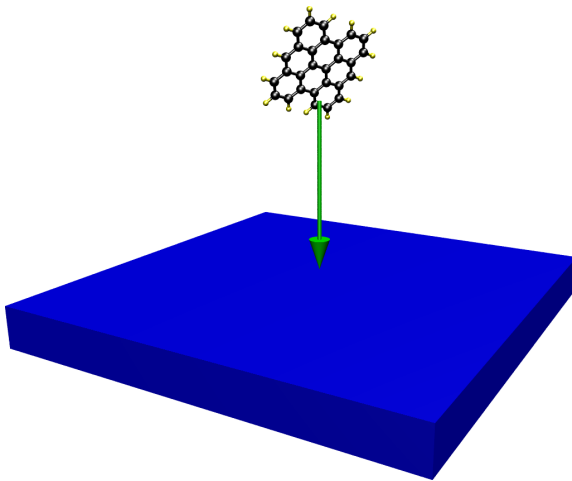
Nanofitas de Grafeno - Caso Zigzag

- Z-GNRs possuem um conjunto de estados magnéticos.

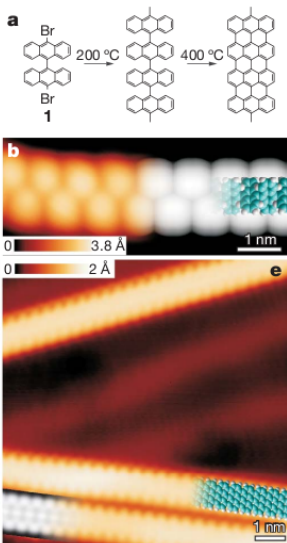


L. Pisani et al., Physical Review B **75**, 064418 (2007).

Reações Assistidas por Superfície

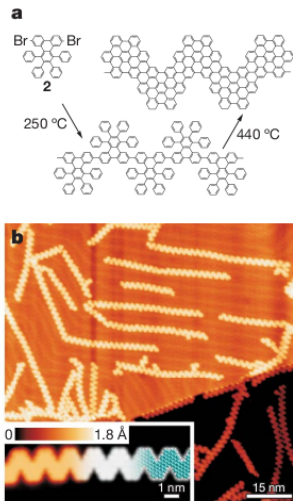
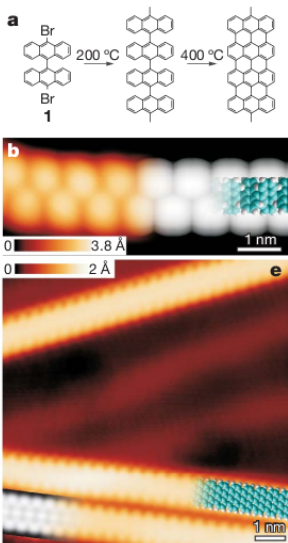


Escolhendo o Precursor



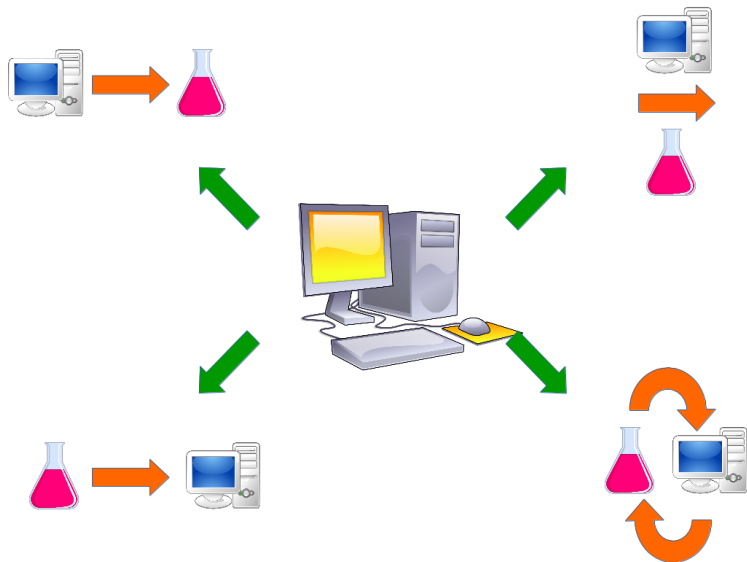
Nature **466**, 470 (2010).

Escolhendo o Precursor

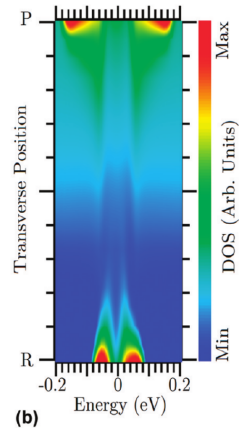
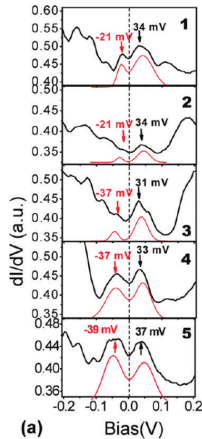
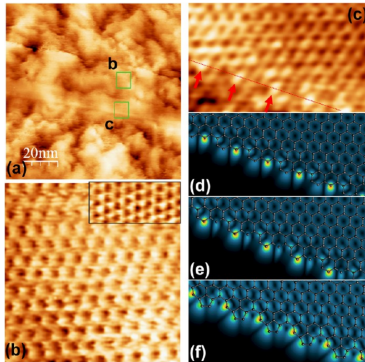


Nature **466**, 470 (2010).

Teoria para que?

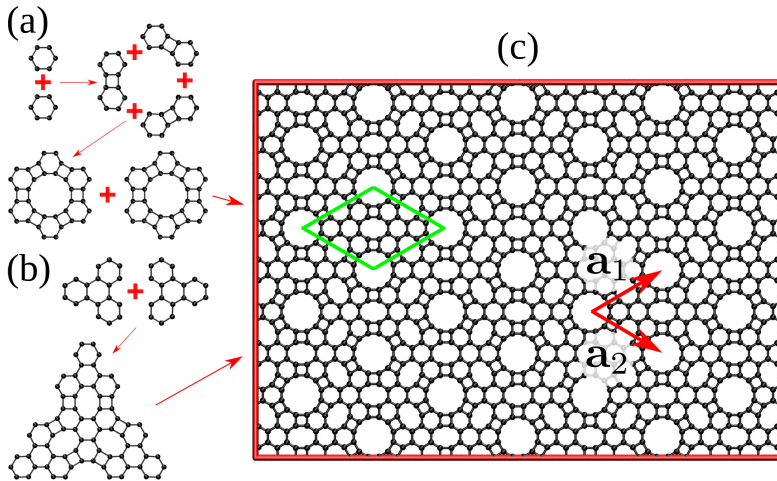


Simulando imagens de microscópio

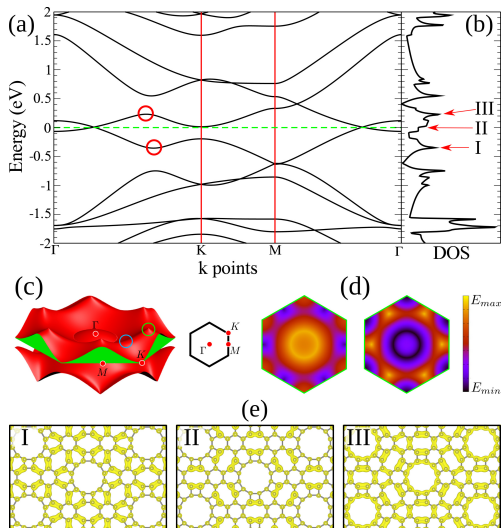


Nano Letters **12**, 1928 (2012).

Montando um “LEGO” Molecular



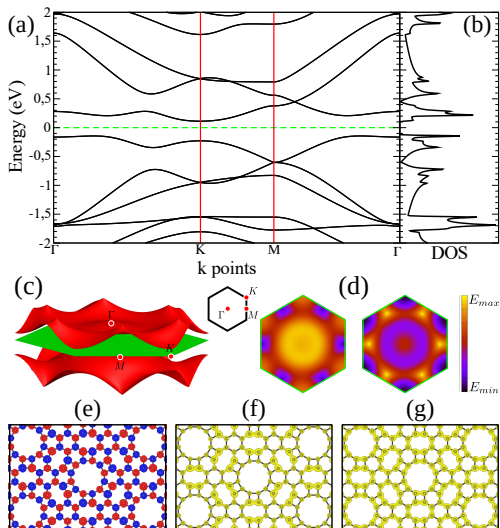
“Sem” spin



PCCP **23**, 25114 (2021).

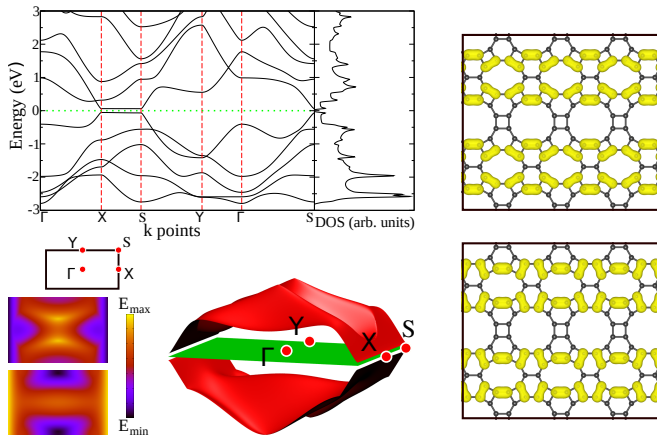
Trifenileno Bidimensional

“Com” spin



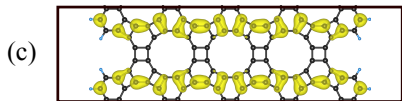
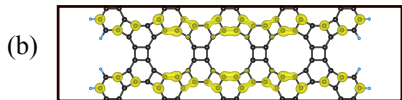
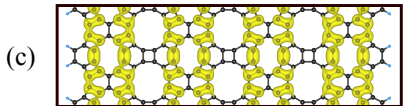
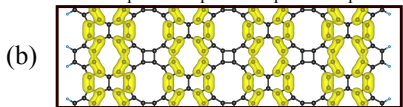
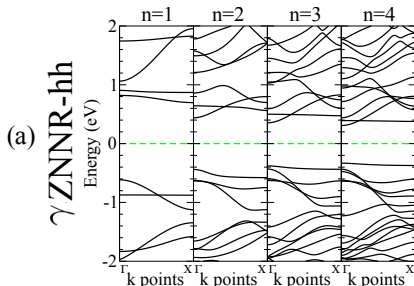
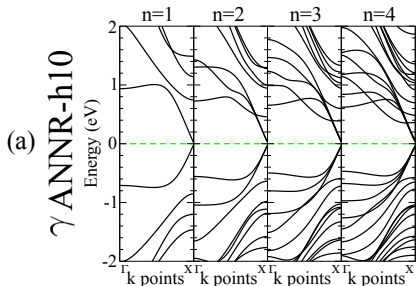
PCCP **23**, 25114 (2021).

Caso γ



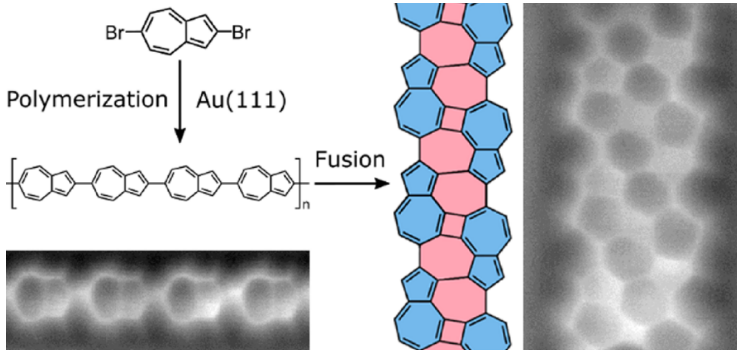
Physical Review Materials **4**, 084003 (2020).

Naftileno- $\gamma \rightarrow$ Nanofitas



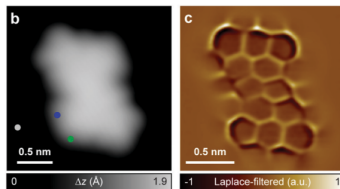
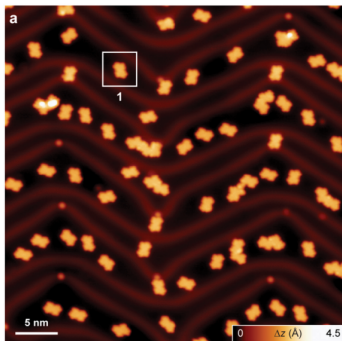
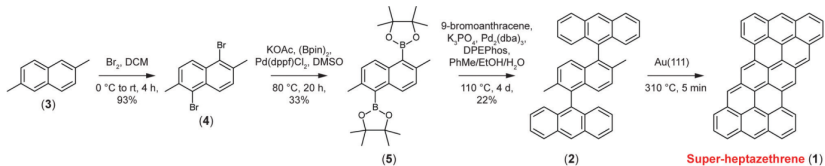
Physical Review Materials **4**, 084003 (2020).

Quadrados em nanocarbonos



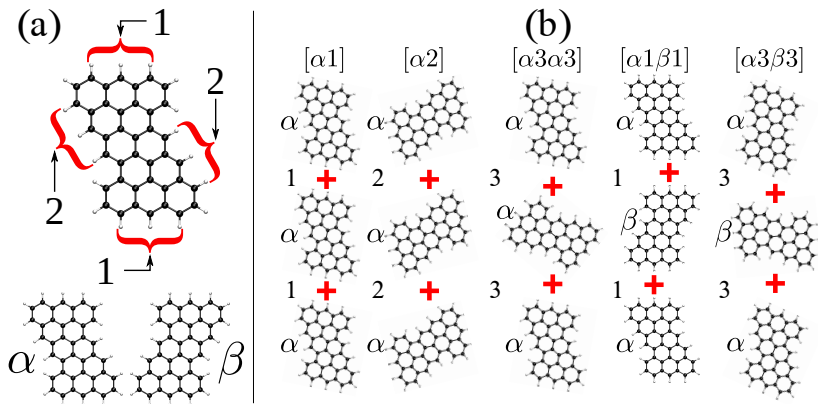
JACS **141**, 17713 (2019).

Super-Hepta-Zetrenos



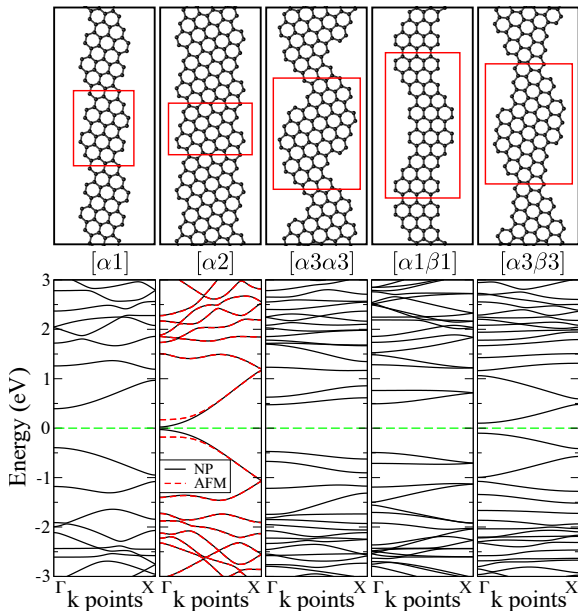
Chem. Commun. **56**, 7467 (2020).

Super-Hepta-Zetrenos

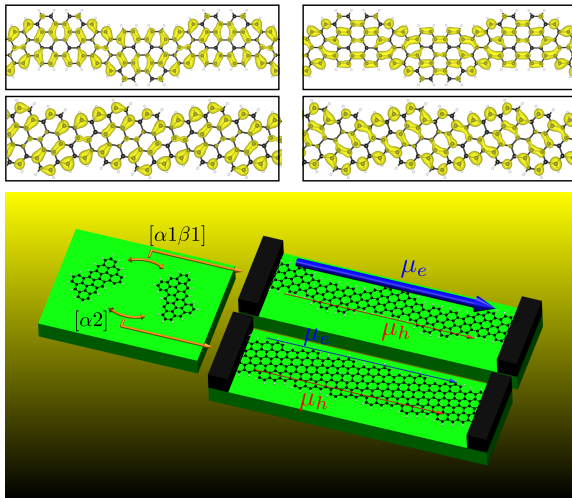


J. Phys. Chem. C **125**, 11235 (2021).

Super-Hepta-Zetrenos

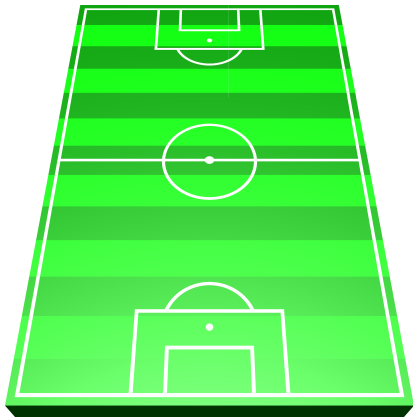


Super-Hepta-Zetrenos



J. Phys. Chem. C **125**, 11235 (2021).

“There is plenty of room at the bottom”



“There is plenty of room at the bottom”

- Experimentos;



“There is plenty of room at the bottom”



- Experimentos;
- Simulações;

“There is plenty of room at the bottom”



- Experimentos;
- Simulações;
- Entender materiais já existentes;

“There is plenty of room at the bottom”



- Experimentos;
- Simulações;
- Entender materiais já existentes;
- Descobrir novos materiais;

“There is plenty of room at the bottom”



- Experimentos;
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- Como conectar peças moleculares...

“There is plenty of room at the bottom”



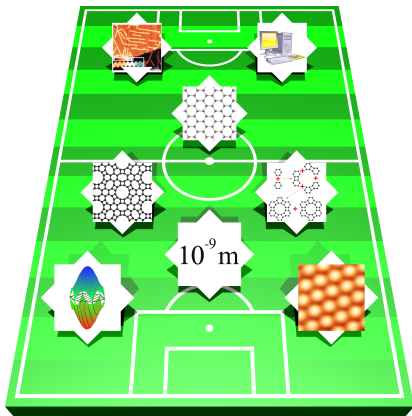
- Experimentos;
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- Descobrir novos materiais;
- Como conectar peças moleculares...
- ... e quais as propriedades resultantes;

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- Experimentos;
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- Nanociência → área prioritária do séc. XXI;

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- Experimentos;
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“There is plenty of room at the bottom”

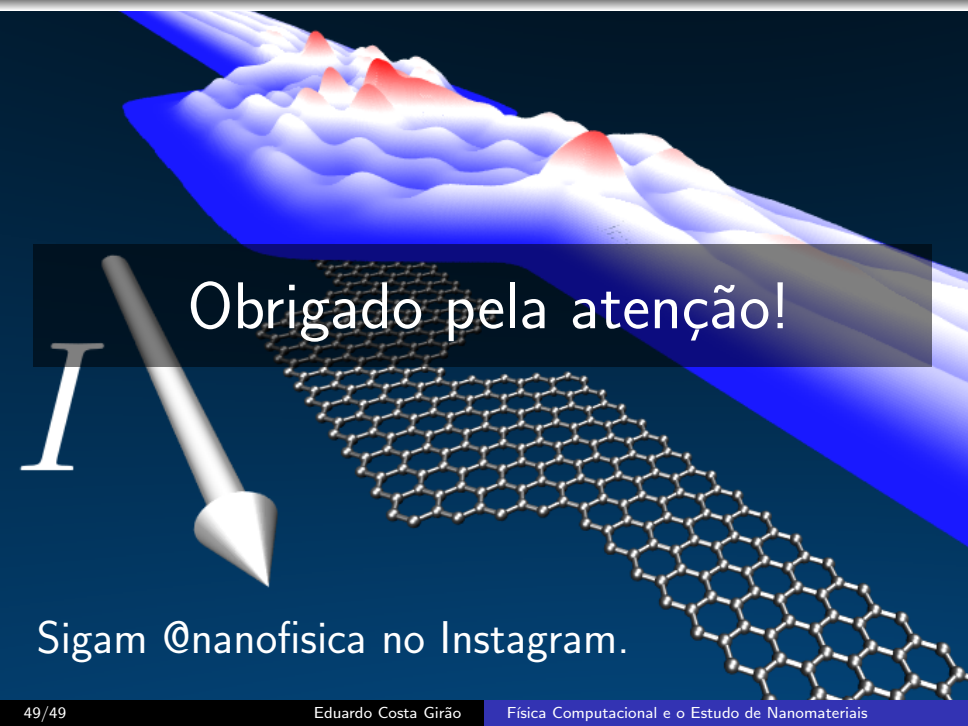


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- Átomos: Instrumento de Trabalho do Físico.



Laboratório de
Simulação
Computacional
Cajuína





Obrigado pela atenção!

Sigam @nanofisica no Instagram.