Curso de Verão

Departamento de Física — UFPE

2024

Recife-PE

22 de **Janeiro** a **09** de **Fevereiro**

FACEPE

SBF — Sociedade Brasileira de Física

CAPES

Minicurso 3:

Materiais Bidimensionais

Prof. Lídia C. Gomes

Dia 1 (29/01)

General introduction.

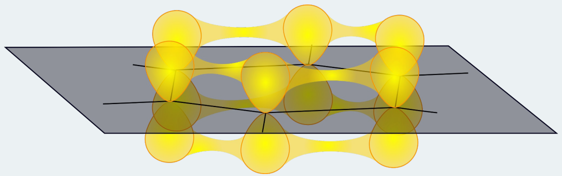
What are 2D materials?

A tiny bit of history.

Some interesting properties.

Dia 2 (30/01)

The origin of dimensionality: an analysis of orbital hybridization in graphene.



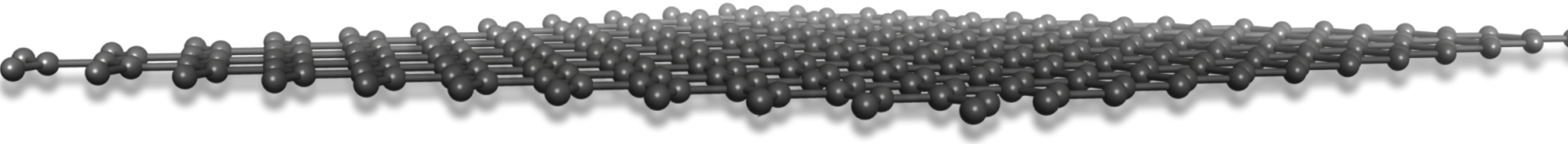
Dia 3 (31/01)

Synthesis methods.

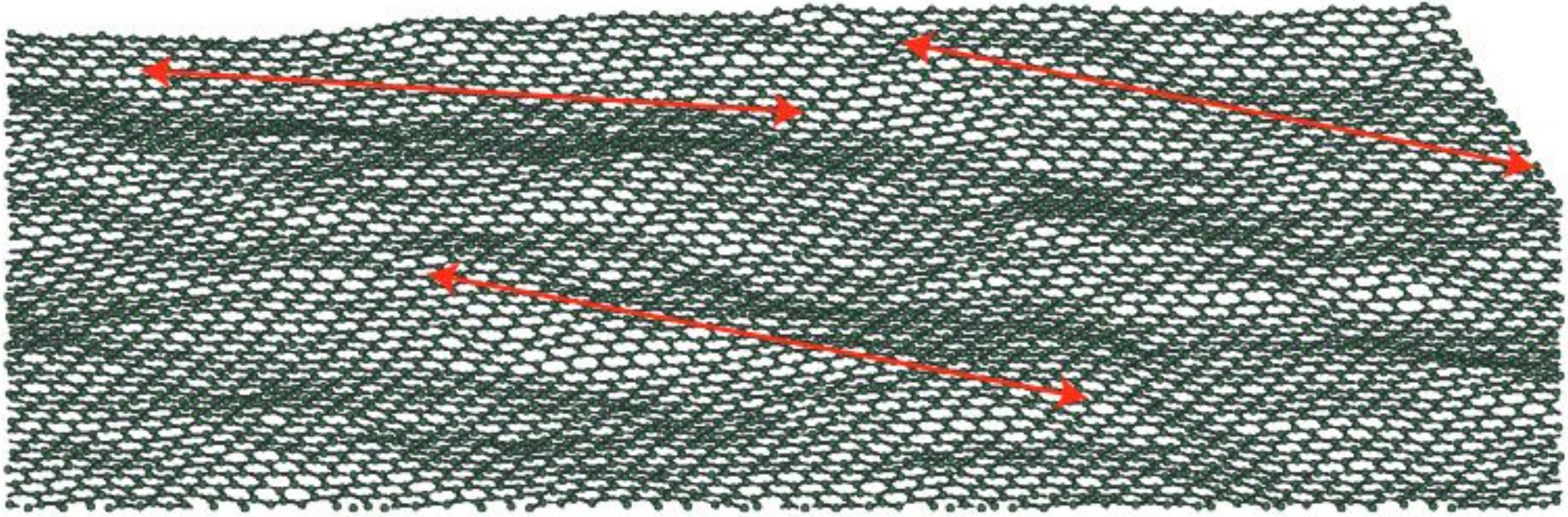
Some experimental achievements.

Some help from computers: ML discovery and development of new 2D materials.

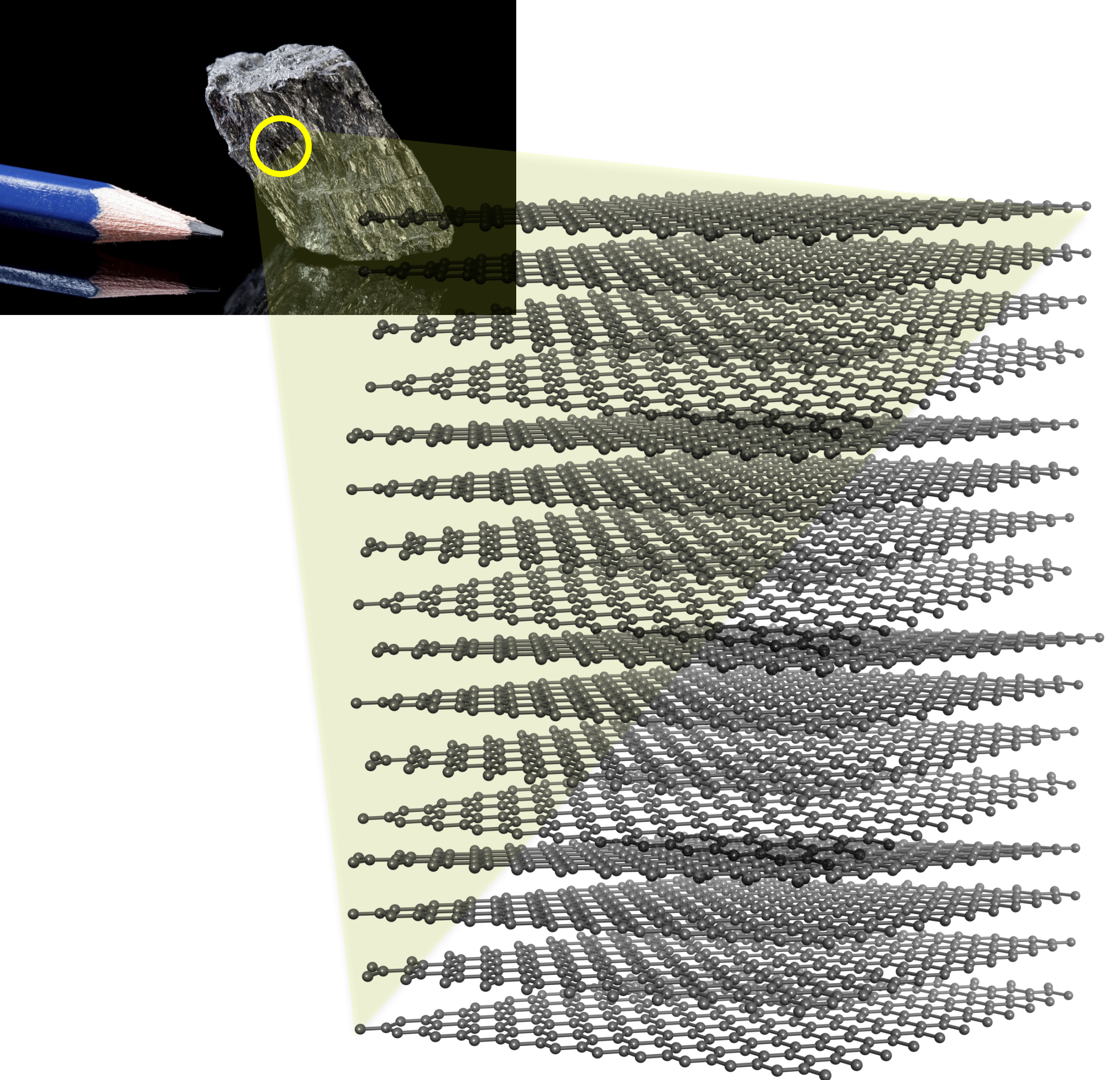
Grafeno



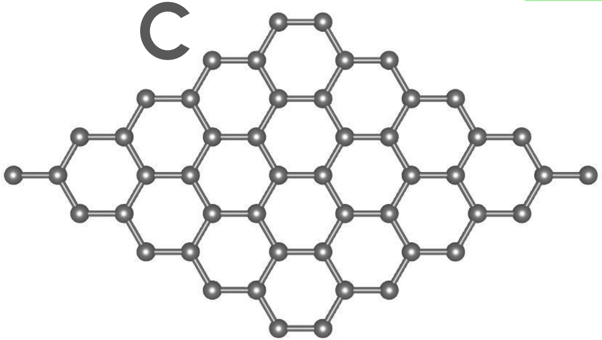
Grafeno

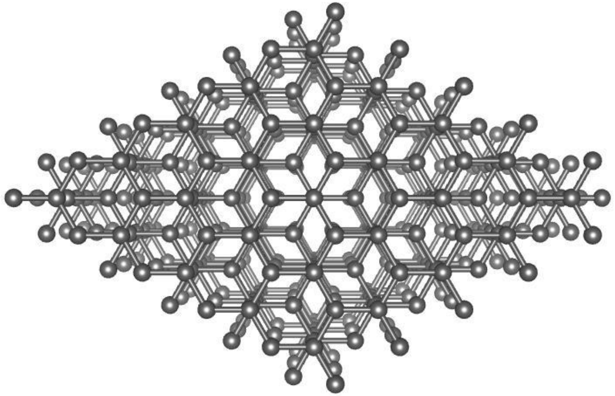


6
C
Carbon
12.011



C





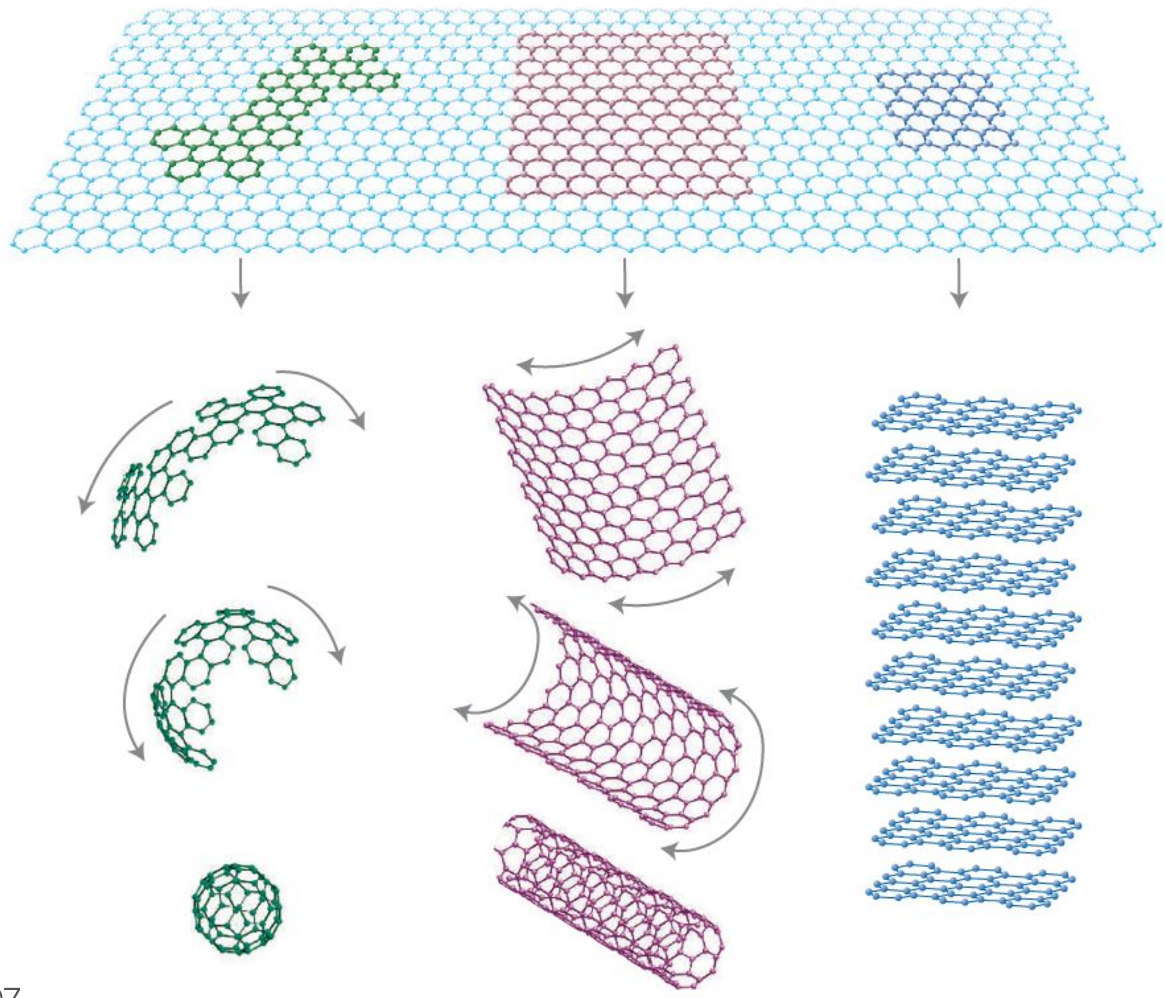
1859 Benjamin Brodie : highly lamellar structure of thermally reduced graphite oxide.

1916 Peter Debye and Paul Scherrer : determination of the structure of graphite by powder X-ray diffraction.

1947 P. R. Wallace : graphene as a starting point for understanding the electronic properties of 3D graphite.

Graphene:

"Mother of all graphitic forms."



K. Novoselov and A. Geim, Nature Mat., 36, 2007

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1961 Hanns-Peter Boehm published a study of extremely thin flakes of graphite, and coined the term "graphene" for the hypothetical single-layer structure.

1984 Gordon Walter Semenoff,[29] and by David P. DiVincenzo and Eugene J. Mele: emergent massless Dirac equation was first pointed. Semenoff emphasized the occurrence in a magnetic field of an electronic Landau level precisely at the Dirac point. This level is responsible for the anomalous integer quantum Hall effect.

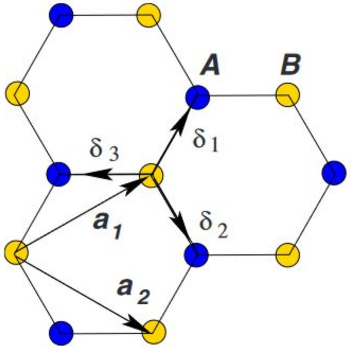
1992 descriptions of carbon nanotubes by R. Saito and Mildred and Gene Dresselhaus in 1992

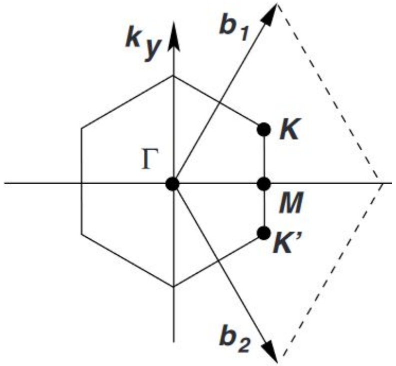
2004 Graphene was properly isolated and characterized in 2004 by Andre Geim and Konstantin Novoselov at the University of Manchester, UK.[

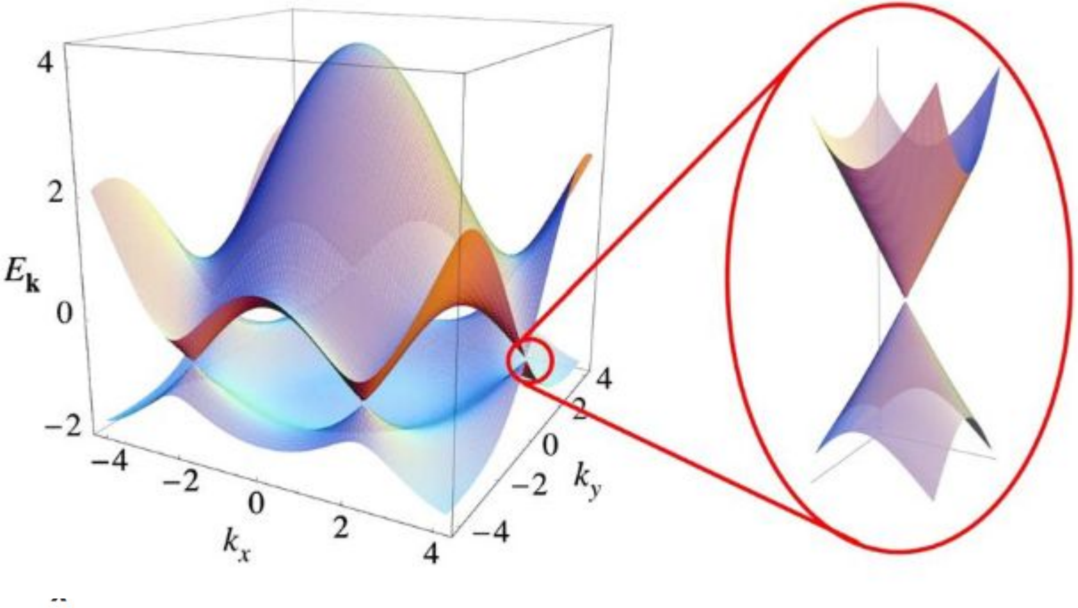
- ***Thinnest.*** At one atom thick, it's the thinnest material we can see.
- ***Lightest.*** One square meter of graphene weighs about 0.77 milligrams. For scale, one square meter of regular paper is 1000 times heavier than graphene and a single sheet of graphene big enough to cover a football field would weigh less than a gram.
- ***Strongest***. Graphene is stronger than steel and Kevlar, with a tensile strength of 10^8 N/cm^2 psi.
- ***Stretchiest***. Graphene has an amazing ability to retain its initial size after strain. Graphene sheets suspended over silicone dioxide cavities had spring constants in the region of 1-5 N/m and a Young's modulus of 0.5 TPa.
- ***Best Conductor of Heat***. At room temperature, graphene's heat conductivity is (4.84±0.44) × 10^3 to (5.30 ±0.48) × 10^3 W·m−1·K−1.
- ***Best Conductor of Electricity***. In graphene, each carbon atom is connected to three other carbon atoms on a two-dimensional plane, which leaves one electron free for electronic conduction. Recent studies have shown electron mobility at values more than 15,000 $cm^2 \cdot V^{-1} \cdot s^{-1}$. Graphene moves electrons 10 times faster than silicon using less energy.
- ***Best Light Absorber***. Graphene can absorb 2.3% of white light, which is remarkable because of its extreme thinness. This means that, once optical intensity reaches saturation fluence, saturable absorption takes place, which makes it possible to achieve full-band mode locking.
- ***Most Renewable.*** Statistically speaking, carbon is the fourth most abundant element in the entire universe (by mass). Because of this abundance, graphene could well be a sustainable, ecologically friendly solution for an increasingly complex world.
- ***Most Exceptional.*** What most captures the imagination is that graphene is one simple material that by itself possesses all these astonishing qualities. No other material in the world is the thinnest, strongest, lightest, and stretchiest, and can conduct heat and electricity super-fast, all at the same time.

https://www.acsmaterial.com/graphene-facts

" One of the most interesting aspects of the graphene problem is that its low-energy excitations are massless, chiral, Dirac fermions. "







Anomalous integer quantum Hall effect (IQHE)

Castro Neto et al, Rev. Mod. Phys., 81, 2009

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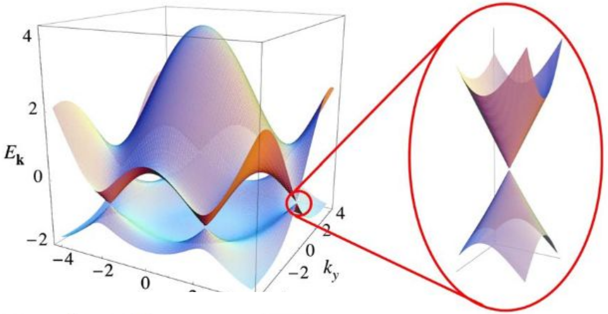
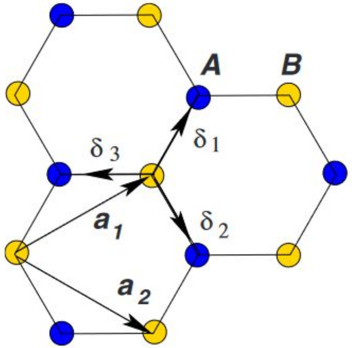
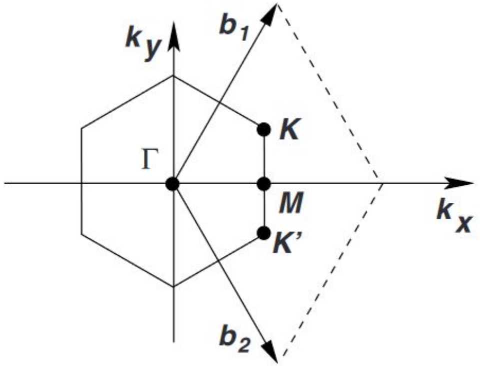
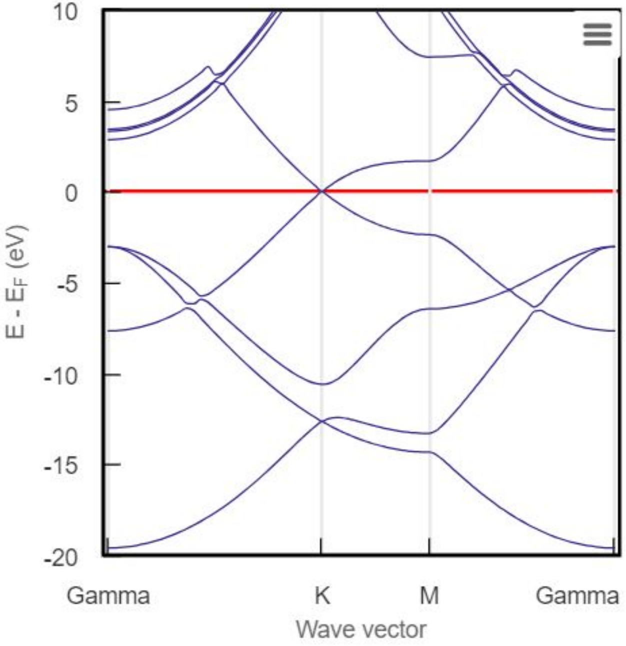








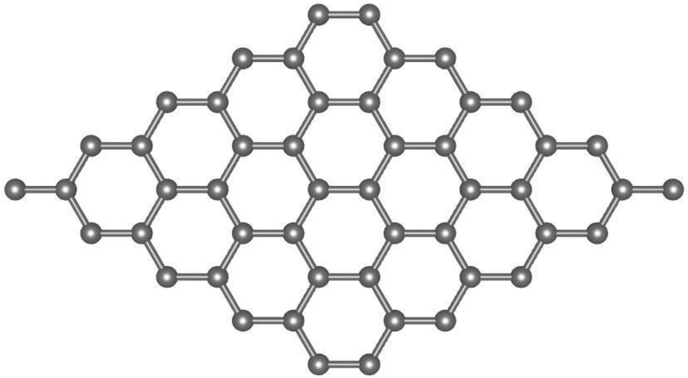
Castro Neto et al, Rev. Mod. Phys., 81, 2009

https://www.materialssquare.com/work/34004

Les Houches Notes on Graphene

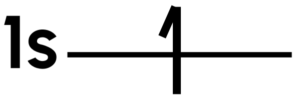
Antonio H. Castro Neto
Department of Physics, Boston University, 590 Commonwealth Avenue, Boston, MA 02215, U.S.A.
(Dated: May 28, 2018)

Graphene research is currently one of the largest fields in condensed matter. Due to its unusual electronic spectrum with Dirac-like quasiparticles, and the fact that it is a unique example of a metallic membrane, graphene has properties that have no match in standard solid state textbooks. In these lecture notes, I discuss some of these properties that are not covered in detail in recent reviews[1]. We study the particular aspects of the physics/chemistry of carbon that influence the properties of graphene; the basic features of graphene's band structure including the π and σ bands; the phonon spectra in free floating graphene; the effects of a substrate on the structural properties of graphene; and the effect of deformations in the propagation of electrons. The objective of these notes is not to provide an unabridged theoretical description of graphene but to point out some of the peculiar aspects of this material.

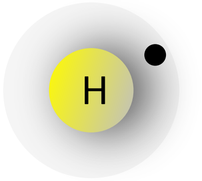


NUS National University of Singapore | Centre for Advanced 2D Materials

Hydrogen atom: **$1s^1$**



$$E_n = -13.6/n^2 \text{ eV}$$



$$Y_\ell^m(\theta,\varphi) = (-1)^m \sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}\, P_\ell^m(\cos\theta)\, e^{im\varphi}$$

$$P_\ell^{-m} = (-1)^m \frac{(\ell-m)!}{(\ell+m)!} P_\ell^m$$

$$Y_0^0(\theta,\varphi) = \frac{1}{2}\sqrt{\frac{1}{\pi}}$$

$$Y_1^{-1}(\theta,\varphi) = \frac{1}{2}\sqrt{\frac{3}{2\pi}}\,\sin\theta\, e^{-i\varphi}$$

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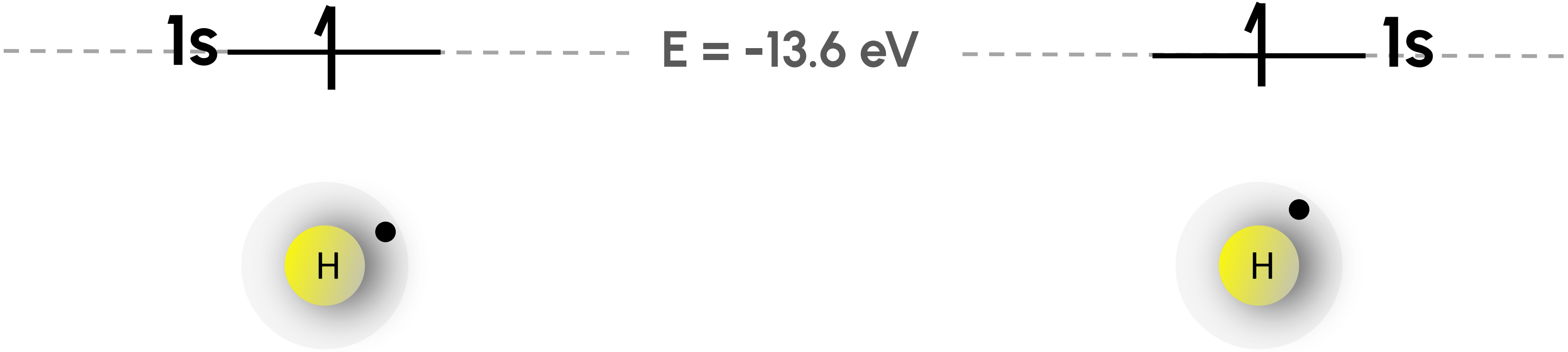
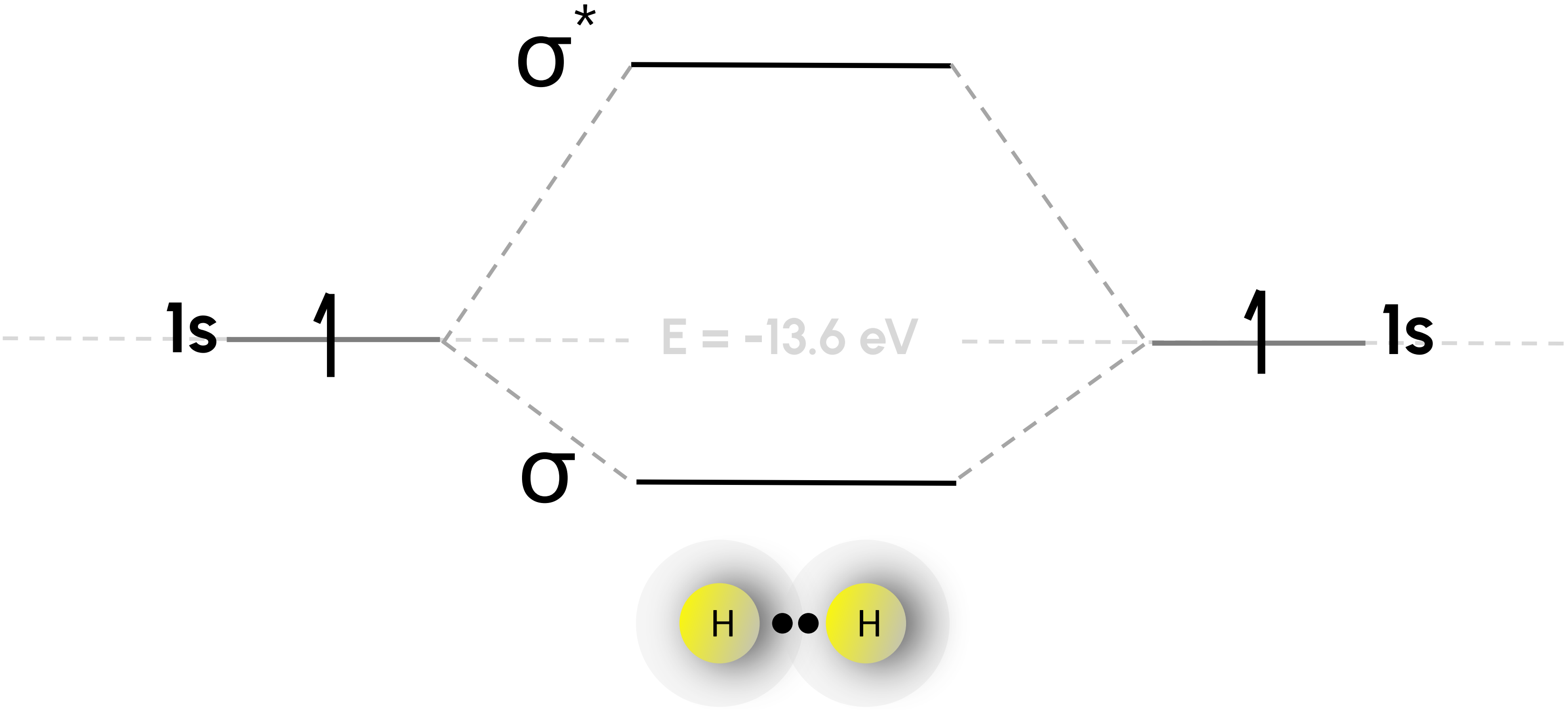
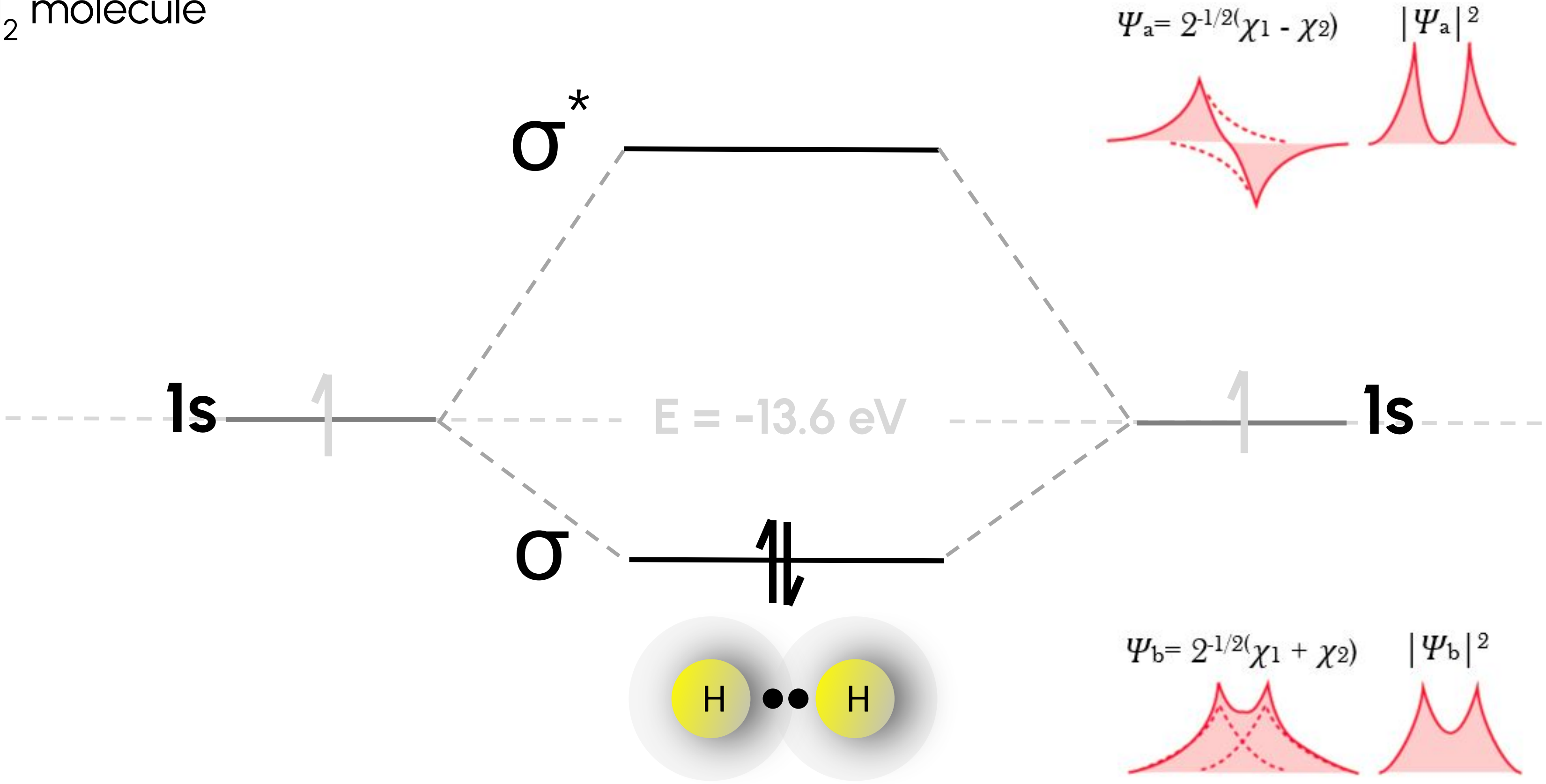


Hydrogen atom: **1s**^{1}

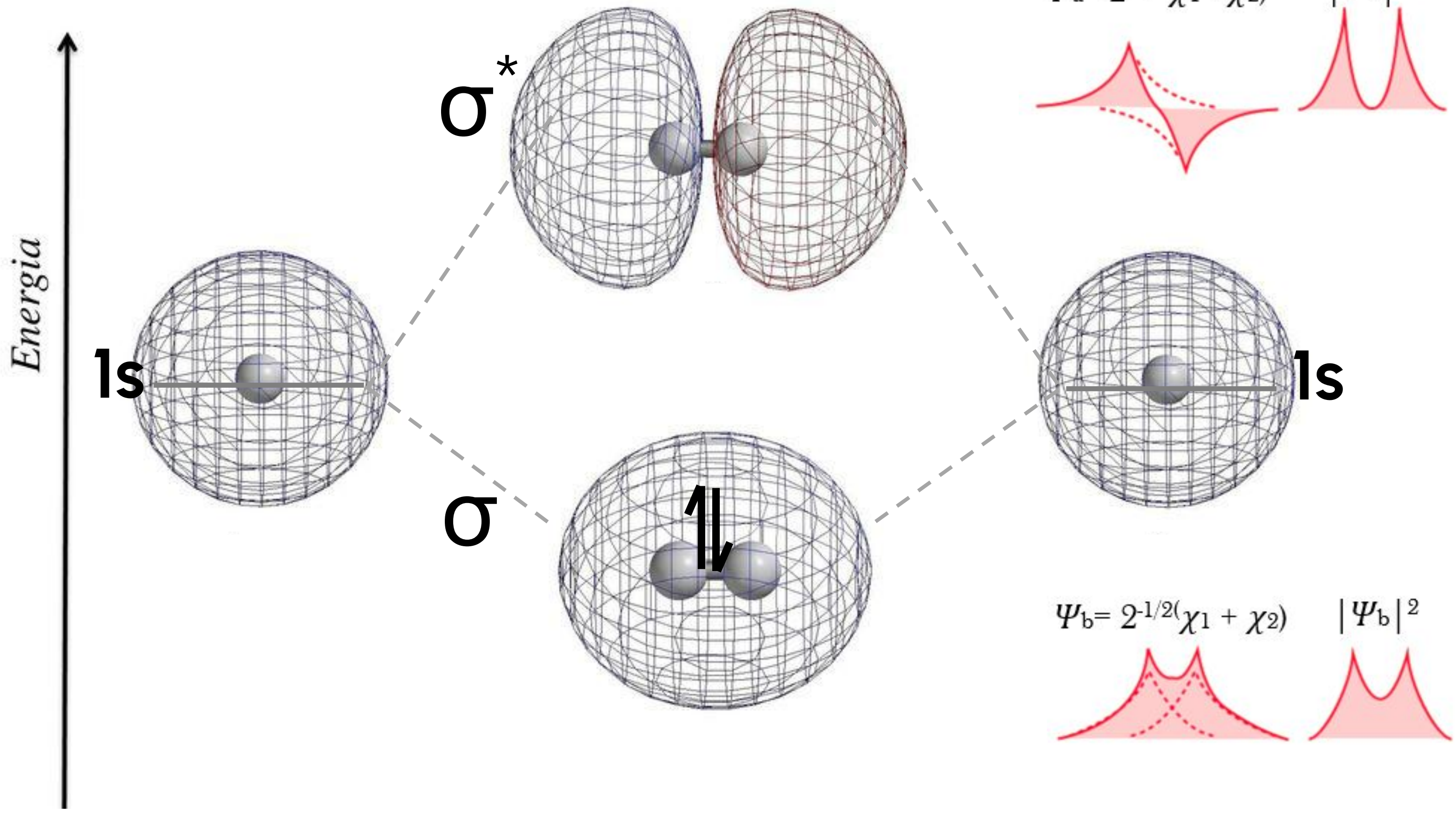


H_2 molecule



$\Psi_a = 2^{-1/2}(\chi_1 - \chi_2)$
$|\Psi_a|^2$
σ*
1s
E = -13.6 eV
1s
σ
H
H
$\Psi_b = 2^{-1/2}(\chi_1 + \chi_2)$
$|\Psi_b|^2$

H_2 molecule



If we consider two carbon atoms: what happens?

Electronic configuration: **$1s^2\ 2s^2\ 2p^2$**

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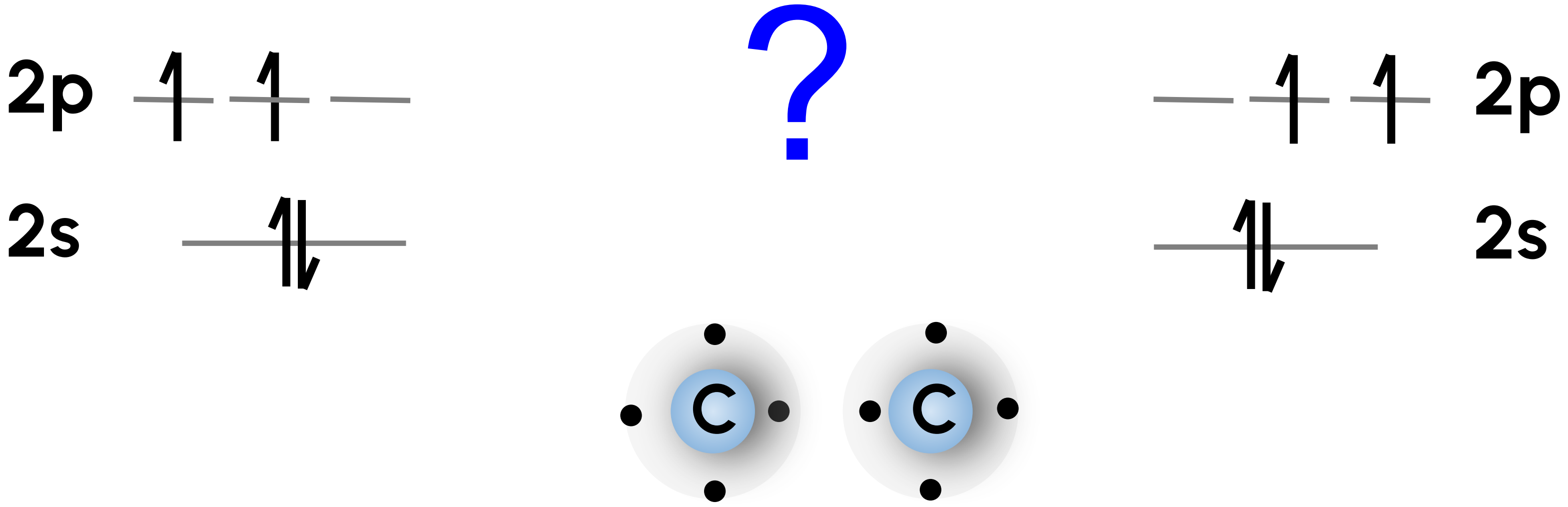
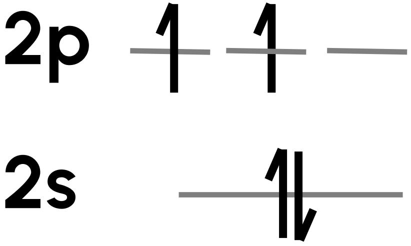
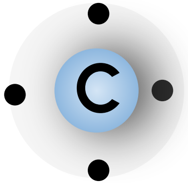
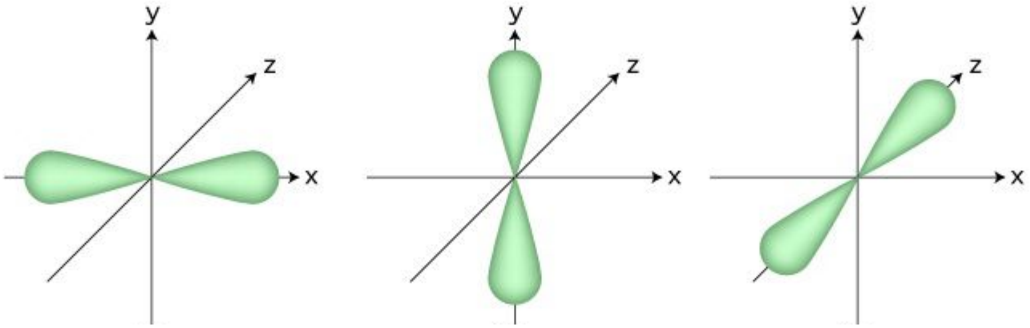


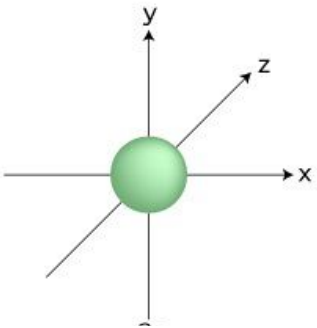
Let's start by looking at one atom only:

Carbon: $\mathbf{1s^2\,2s^2\,2p^2}$









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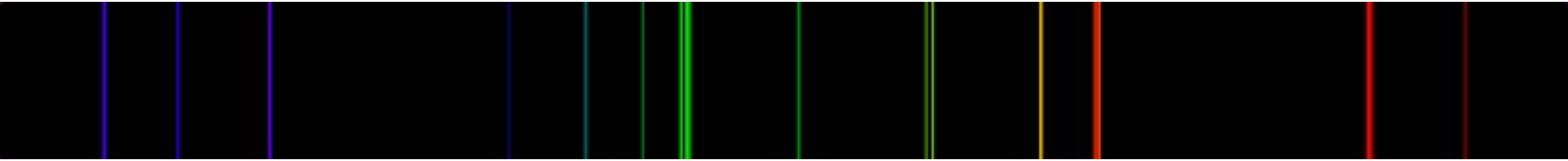
Espectro Atômico

Hydrogen

Carbon

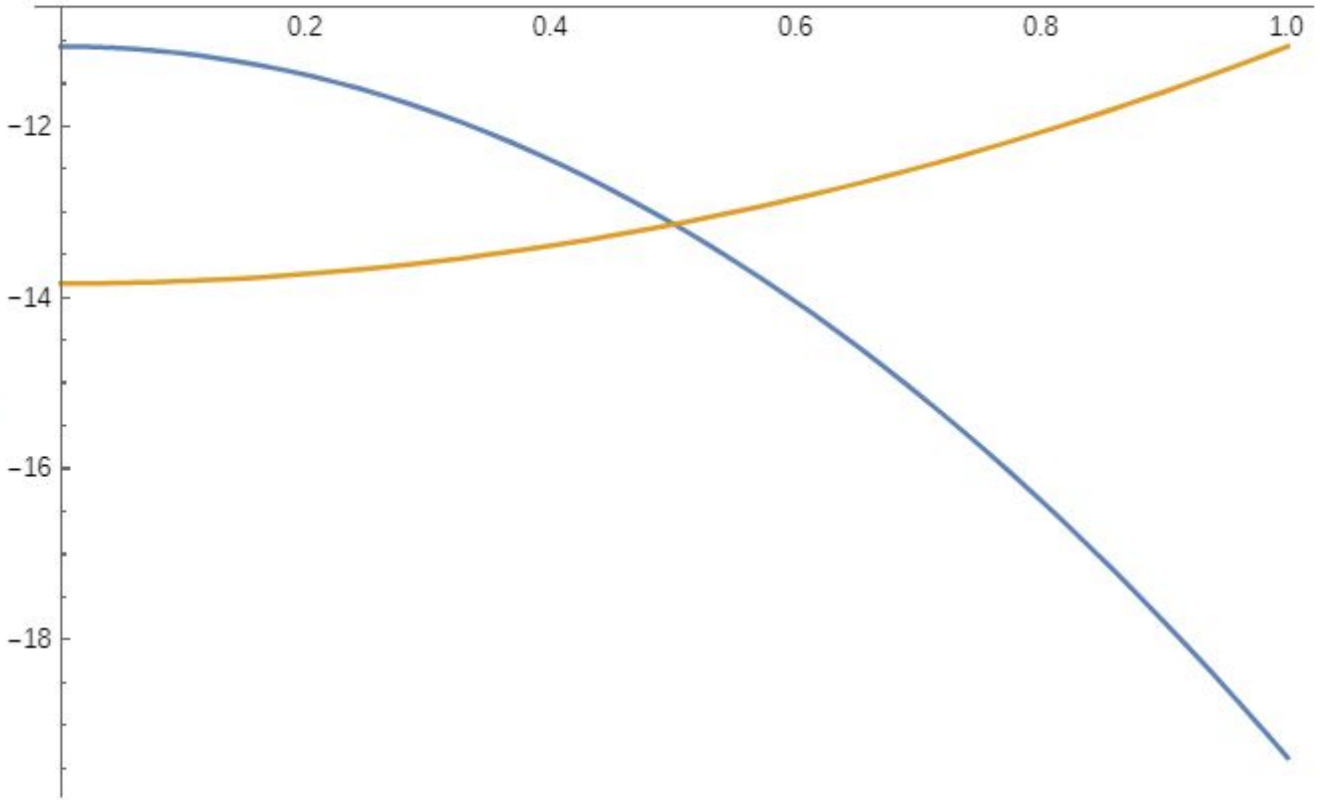


https://www.astronomy.ohio-state.edu/pogge.1/TeachRes/HandSpec/ato

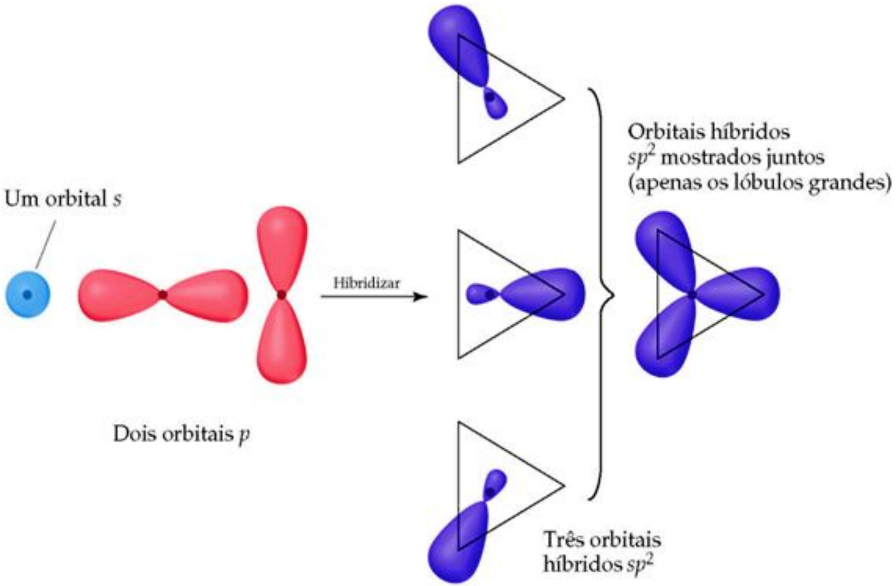
```
In[1]:= Es = -19.38;
        Ep = -11.07;

In[5]:= Plot[{x^2 * Es + (1 - x^2) * Ep, (1 - x^2) Es / 3 + (2 + x^2) Ep / 3}, {x, 0, 1}]
```

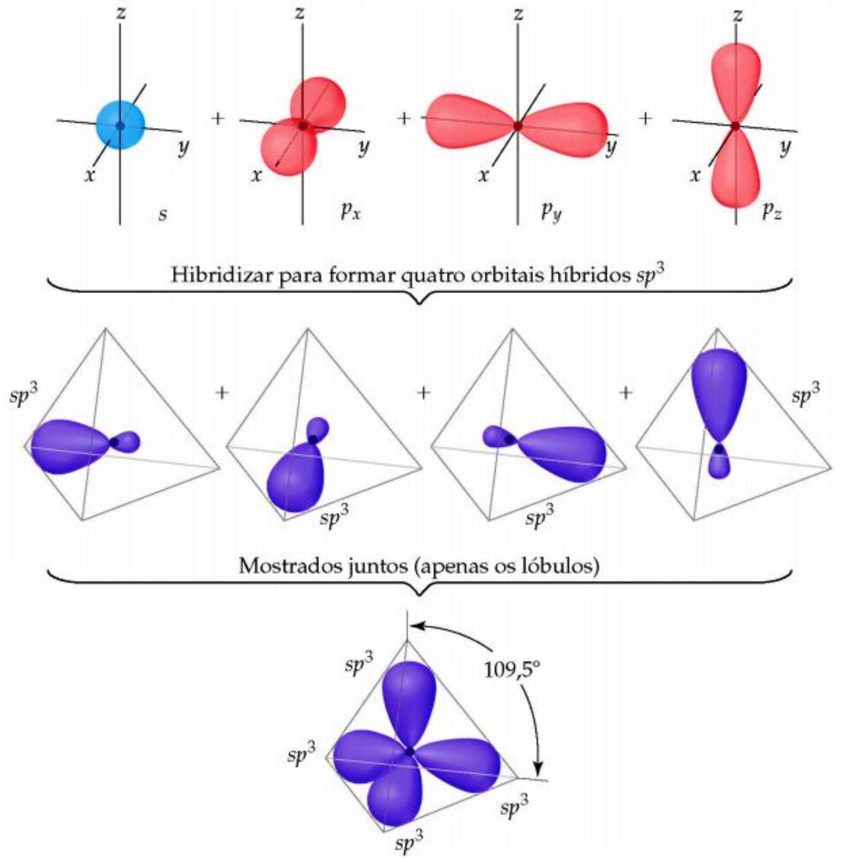
Out[5]=



A = 0
sp^2



A = 1/2
sp^3



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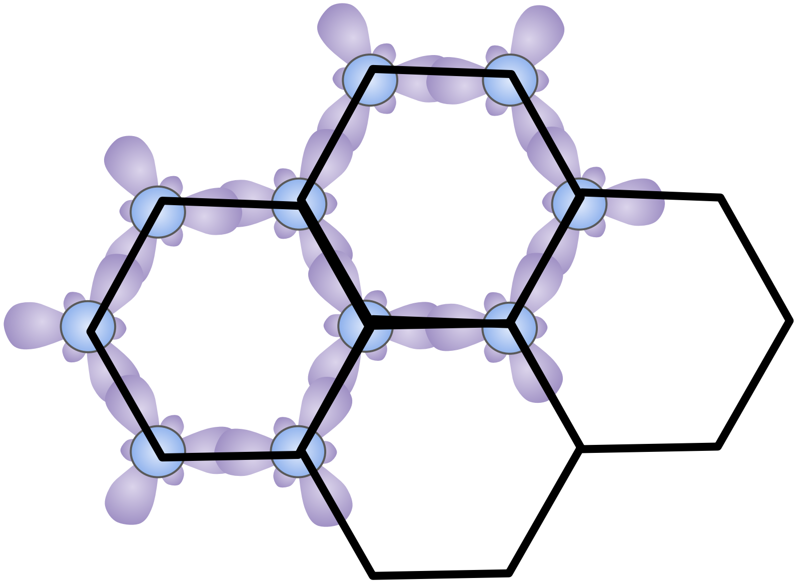
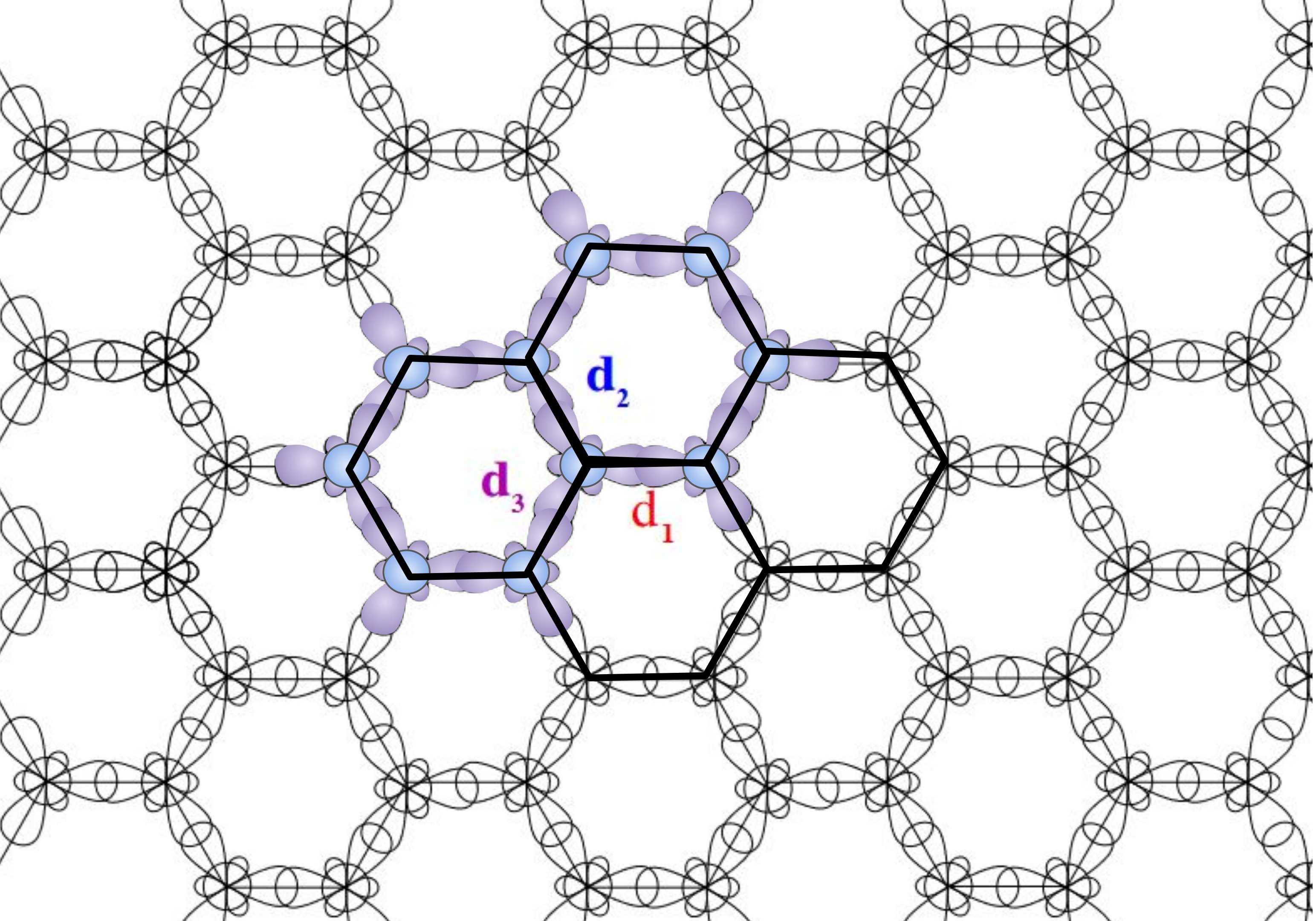
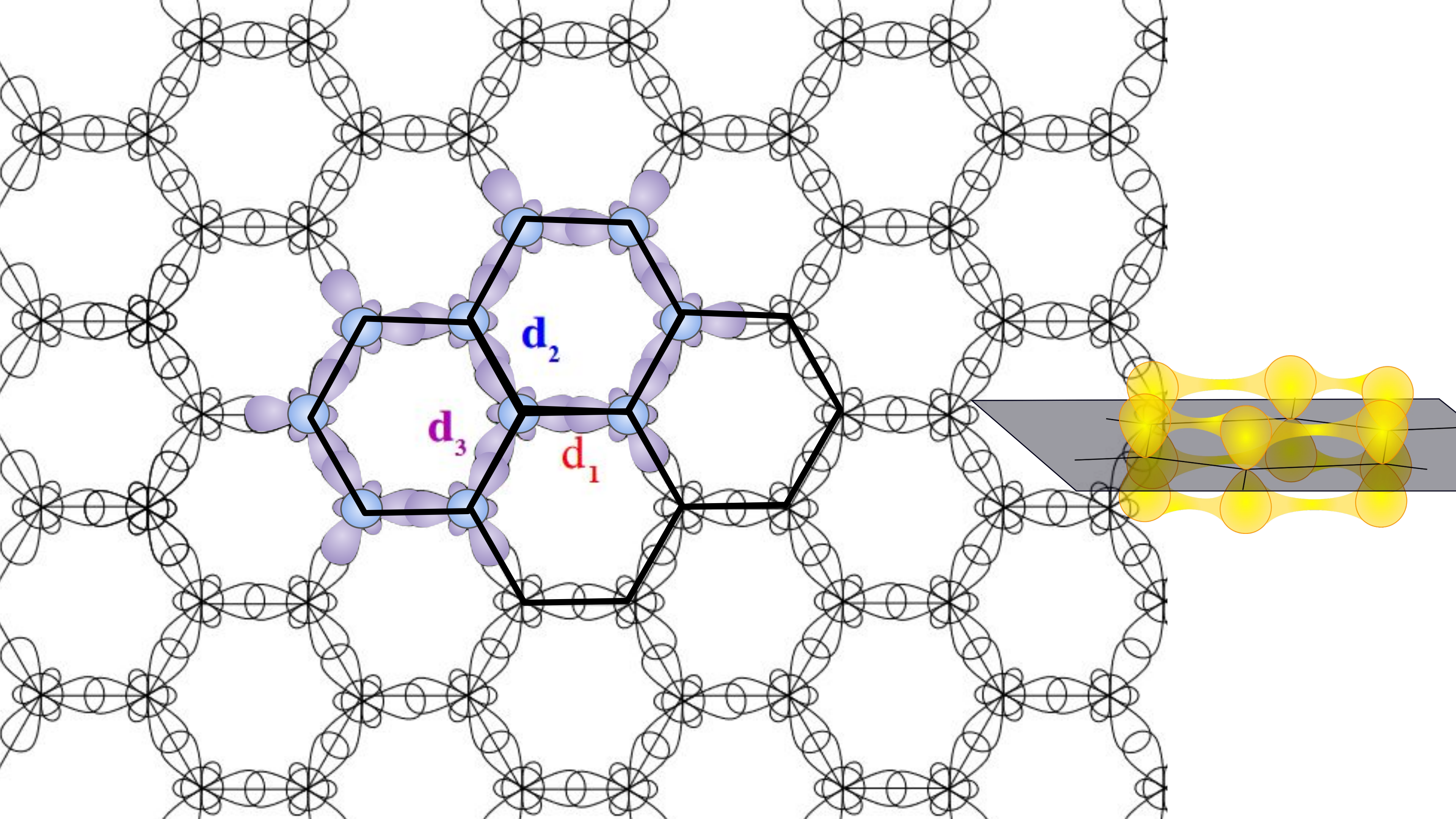
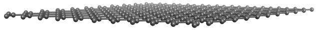
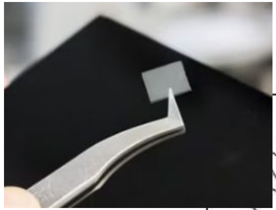


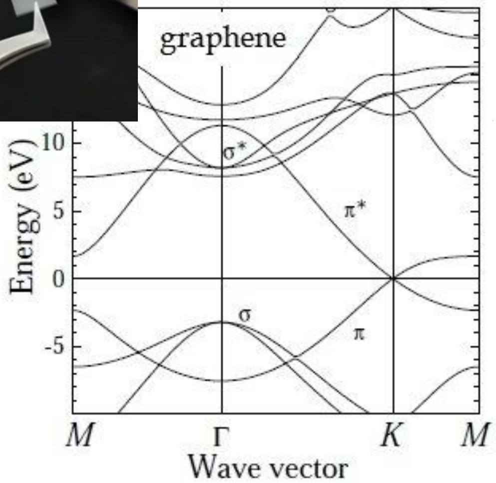

d2
d3
d1


d2
d3
d1

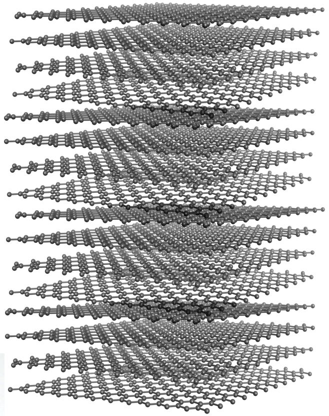
Grafeno

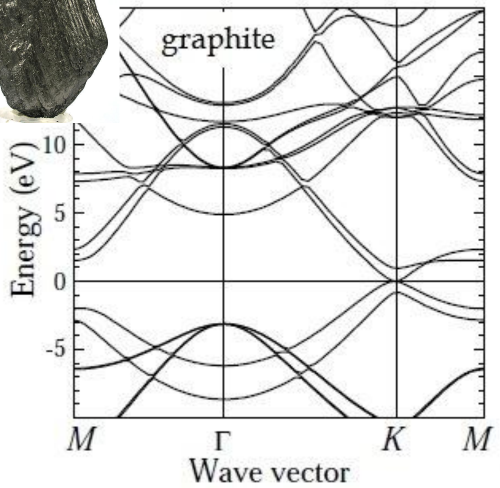




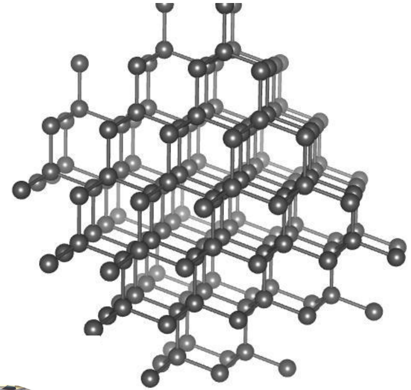


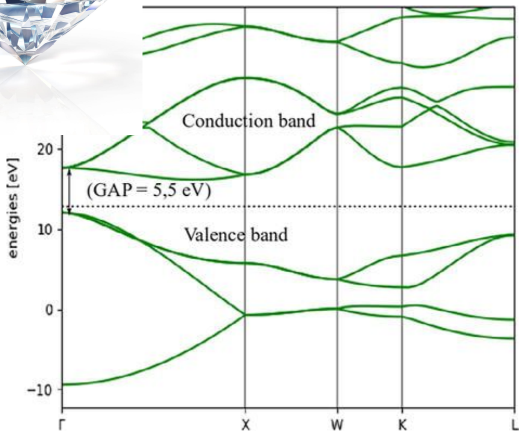
Grafite



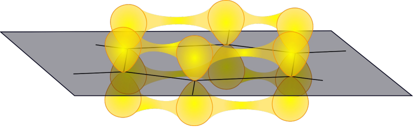


Diamante





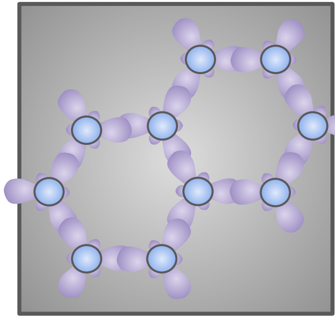
https://www.intechopen.com/chapters/86



$$p_z$$

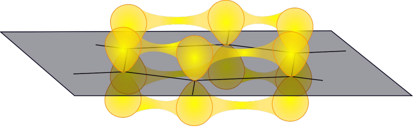
$$[H] = \begin{bmatrix} \epsilon_\pi & V_{pp\pi}\gamma_{\mathbf{k}} & 0 & 0 & 0 & 0 & 0 & 0 \\ V_{pp\pi}\gamma^*_{\mathbf{k}} & \epsilon_\pi & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \epsilon_\sigma & V_\sigma e^{i\mathbf{k}\cdot\vec{\delta}_1} & V_{\text{intra}} & 0 & V_{\text{intra}} & 0 \\ 0 & 0 & V_\sigma e^{-i\mathbf{k}\cdot\vec{\delta}_1} & \epsilon_\sigma & 0 & V_{\text{intra}} & 0 & V_{\text{intra}} \\ 0 & 0 & V_{\text{intra}} & 0 & \epsilon_\sigma & V_\sigma e^{i\mathbf{k}\cdot\vec{\delta}_2} & V_{\text{intra}} & 0 \\ 0 & 0 & 0 & V_{\text{intra}} & V_\sigma e^{-i\mathbf{k}\cdot\vec{\delta}_2} & \epsilon_\sigma & 0 & V_{\text{intra}} \\ 0 & 0 & V_{\text{intra}} & 0 & V_{\text{intra}} & 0 & \epsilon_\sigma & V_\sigma e^{i\mathbf{k}\cdot\vec{\delta}_3} \\ 0 & 0 & 0 & V_{\text{intra}} & 0 & V_{\text{intra}} & V_\sigma e^{-i\mathbf{k}\cdot\vec{\delta}_3} & \epsilon_\sigma \end{bmatrix}$$

$$sp^2$$



$$\begin{aligned} H \;=\; & \epsilon_\pi \sum_{n,a} c^\dagger_{n,a,0} c_{n,a,0} + \epsilon_\sigma \sum_{n,a,i\neq 0} c^\dagger_{n,a,i} c_{n,a,i} + V_{\text{intra}} \sum_{n,a,i\neq j\neq 0} (c^\dagger_{n,a,i} c_{n,a,j} + \text{h.c.}) \\ & + V_{pp\pi} \sum_{\langle n,m\rangle} (c^\dagger_{n,A,0} c_{m,B,0} + \text{h.c.}) + V_\sigma \sum_{\langle n,m\rangle, i\neq 0} (c^\dagger_{n,A,i} c_{m,B,i} + \text{h.c.})\,. \end{aligned}$$

A. H. Castro Neto, Les Houches Notes on Graphene, 2010



p_z

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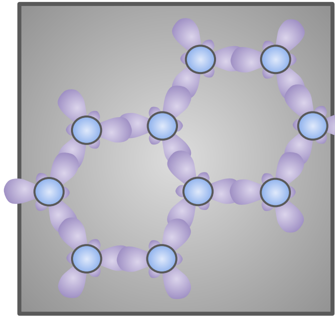
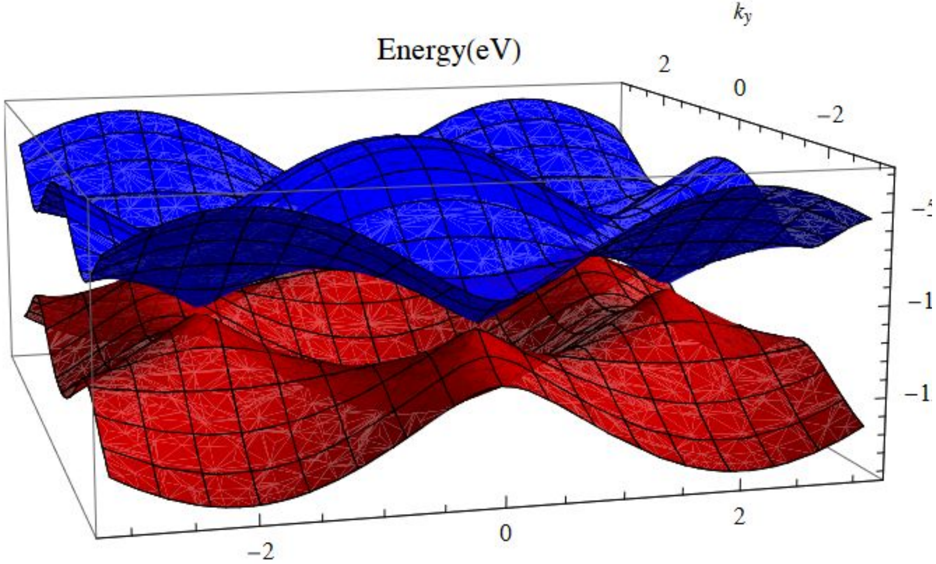
sp^2

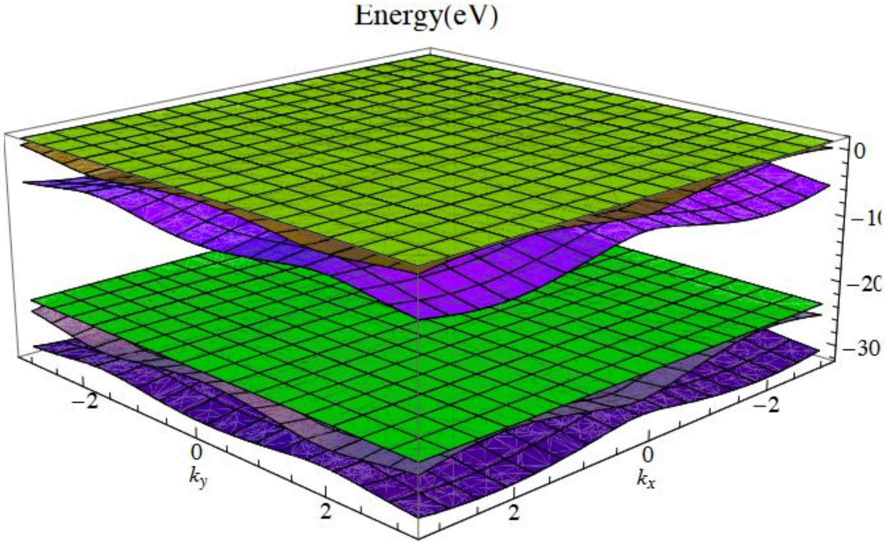


$$\begin{aligned} E_{\pi,\pm}(\mathbf{k}) &= \epsilon_\pi \pm |V_{pp\pi}||\gamma_{\mathbf{k}}|\,, \\ E_{\sigma,1,\pm}(\mathbf{k}) &= \epsilon_\sigma - V_{\text{intra}} \pm V_\sigma\,, \\ E_{\sigma,2,\pm}(\mathbf{k}) &= \epsilon_\sigma + \frac{V_{\text{intra}}}{2} + \sqrt{\left(\frac{3V_{\text{intra}}}{2}\right)^2 + V_\sigma^2 \pm |V_{\text{intra}}V_\sigma||\gamma_{\mathbf{k}}|} \\ E_{\sigma,3,\pm}(\mathbf{k}) &= \epsilon_\sigma + \frac{V_{\text{intra}}}{2} - \sqrt{\left(\frac{3V_{\text{intra}}}{2}\right)^2 + V_\sigma^2 \pm |V_{\text{intra}}V_\sigma||\gamma_{\mathbf{k}}|} \end{aligned}$$

A. H. Castro Neto, Les Houches Notes on Graphene, 2010

$$
\begin{aligned}
E_{\pi,\pm}(\mathbf{k}) &= \epsilon_\pi \pm |V_{pp\pi}||\gamma_\mathbf{k}| \,, \\
E_{\sigma,1,\pm}(\mathbf{k}) &= \epsilon_\sigma - V_{\text{intra}} \pm V_\sigma \,, \\
E_{\sigma,2,\pm}(\mathbf{k}) &= \epsilon_\sigma + \frac{V_{\text{intra}}}{2} + \sqrt{\left(\frac{3V_{\text{intra}}}{2}\right)^2 + V_\sigma^2 \pm |V_{\text{intra}}V_\sigma||\gamma_\mathbf{k}|} \\
E_{\sigma,3,\pm}(\mathbf{k}) &= \epsilon_\sigma + \frac{V_{\text{intra}}}{2} - \sqrt{\left(\frac{3V_{\text{intra}}}{2}\right)^2 + V_\sigma^2 \pm |V_{\text{intra}}V_\sigma||\gamma_\mathbf{k}|}
\end{aligned}
$$





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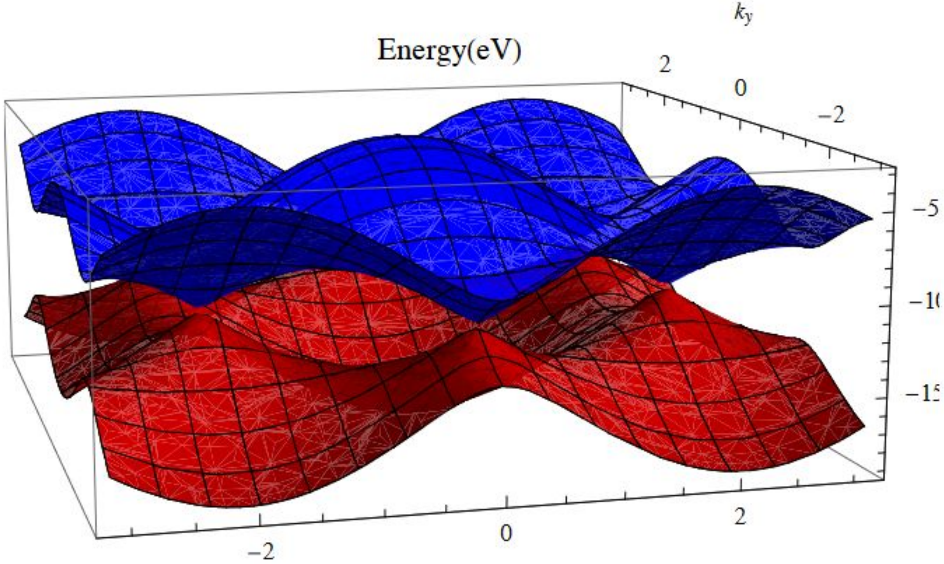
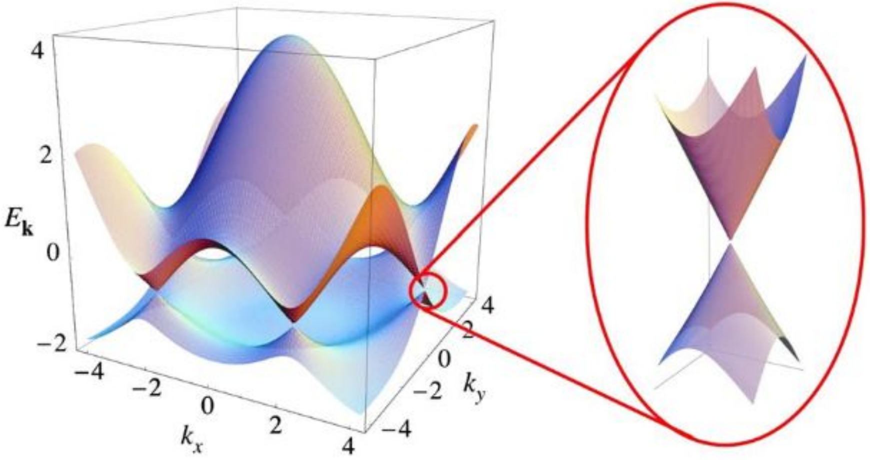
$$E_{\pi,\pm}(\mathbf{k}) = \epsilon_\pi \pm |V_{pp\pi}||\gamma_\mathbf{k}|,$$

$$|\gamma_\mathbf{k}| = \sqrt{3 + 2\cos(\mathbf{k}\cdot(\vec{\delta}_1 - \vec{\delta}_2)) + 2\cos(\mathbf{k}\cdot(\vec{\delta}_1 - \vec{\delta}_3)) + 2\cos(\mathbf{k}\cdot(\vec{\delta}_2 - \vec{\delta}_3))}\,.$$

$$V_{pp\pi}\ (\approx -2.4\ \text{eV for}\ \ell = 1.42\ \text{Å})$$





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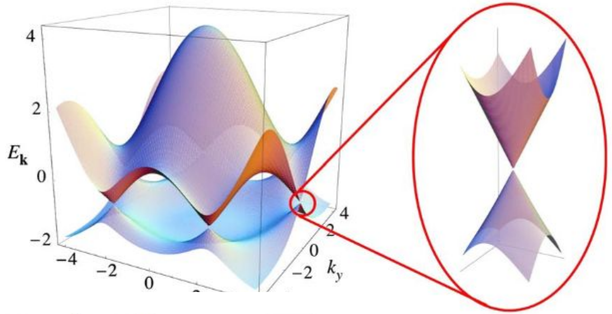
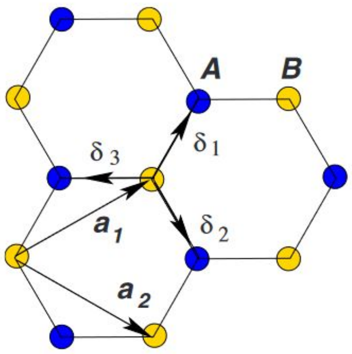
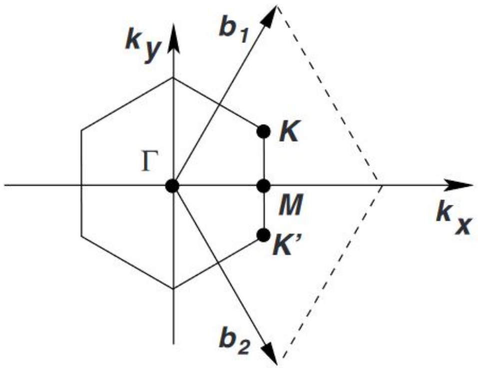
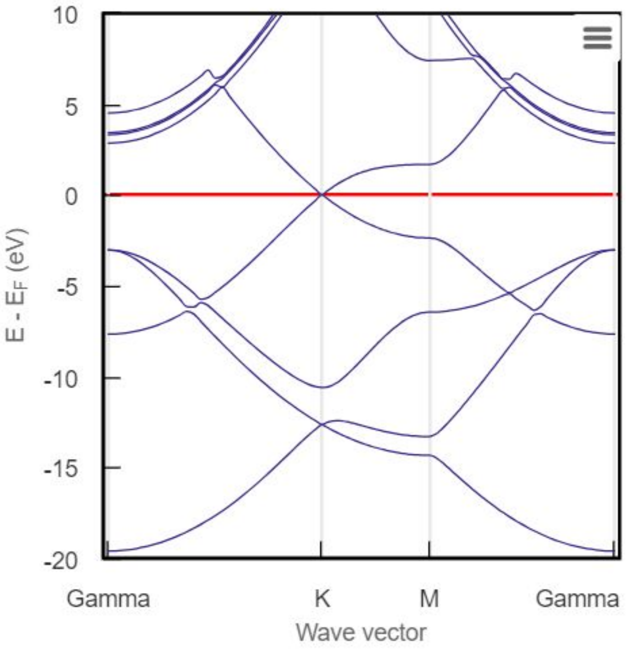
" One of the most interesting aspects of the graphene problem is that its low-energy excitations are massless, chiral, Dirac fermions. "



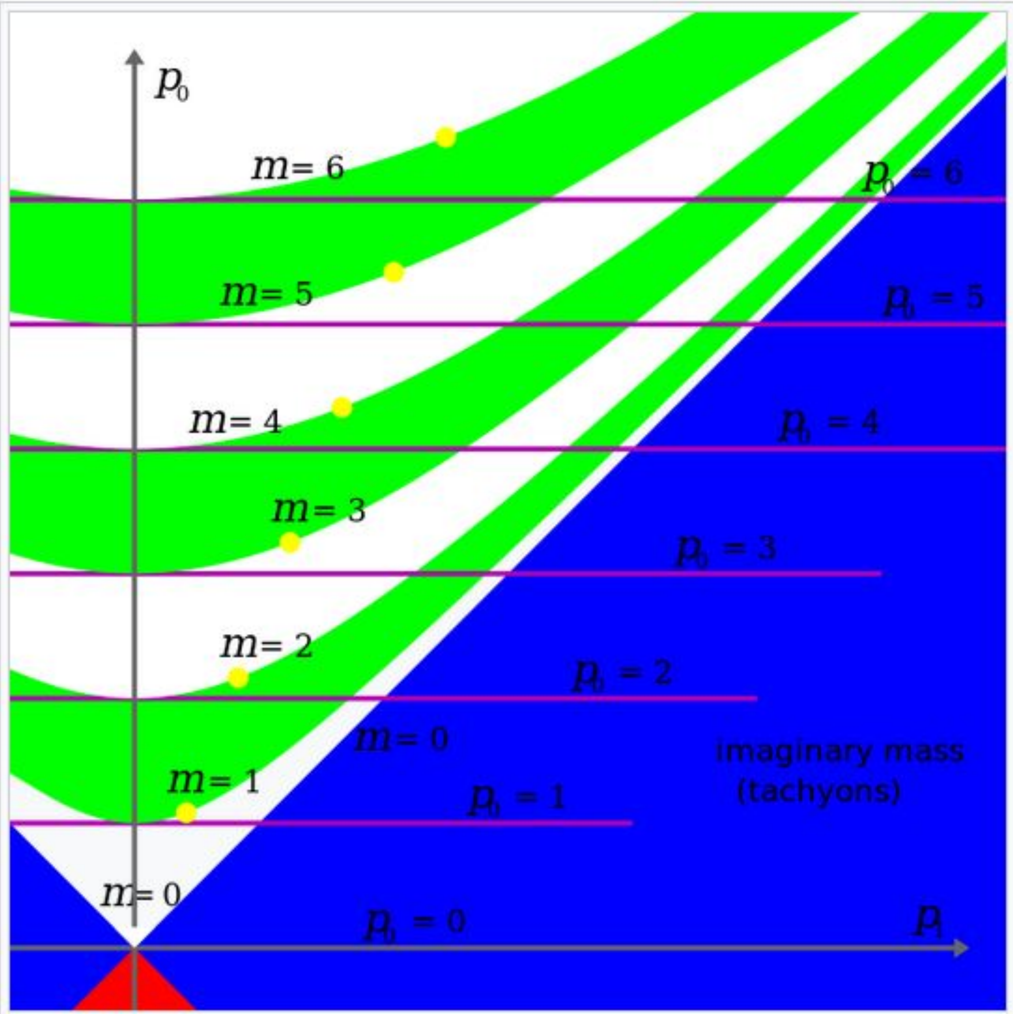






Castro Neto et al, Rev. Mod. Phys., 81, 2009

https://www.materialssquare.com/work/34004



p_0
$m = 6$
$p_0 = 6$
$m = 5$
$p_0 = 5$
$m = 4$
$p_0 = 4$
$m = 3$
$p_0 = 3$
$m = 2$
$p_0 = 2$
$m = 0$
imaginary mass
(tachyons)
$m = 1$
$p_0 = 1$
$m = 0$
$p_0 = 0$
p_1