Transporte electrónico en sistemas bidimensionales

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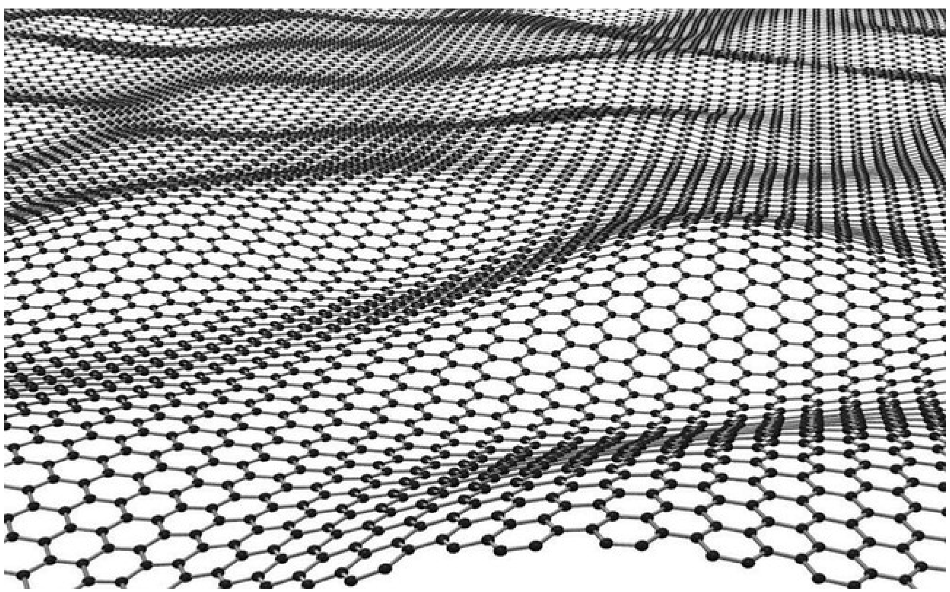
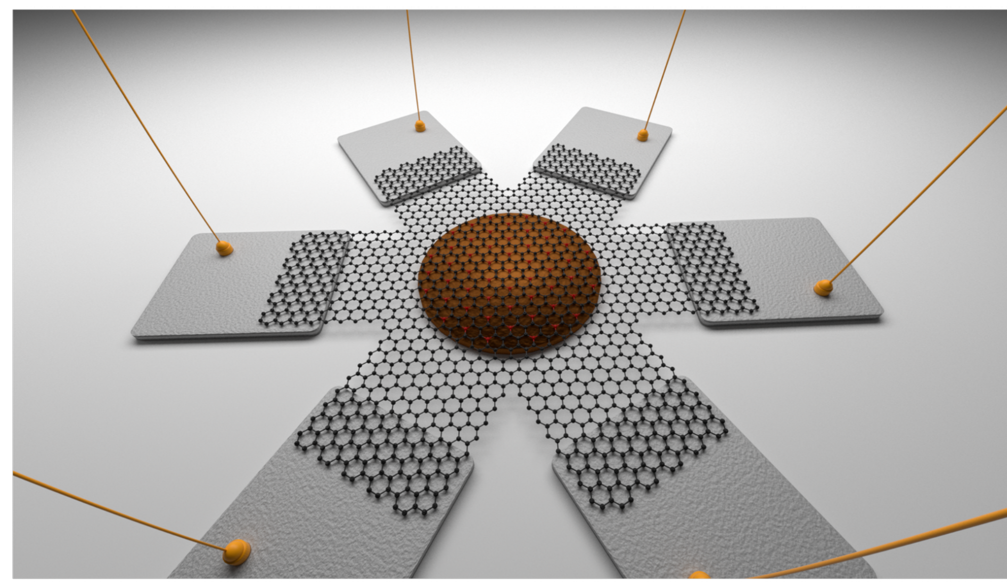
Depto. Física y Química Teórica, FQ-UNAM

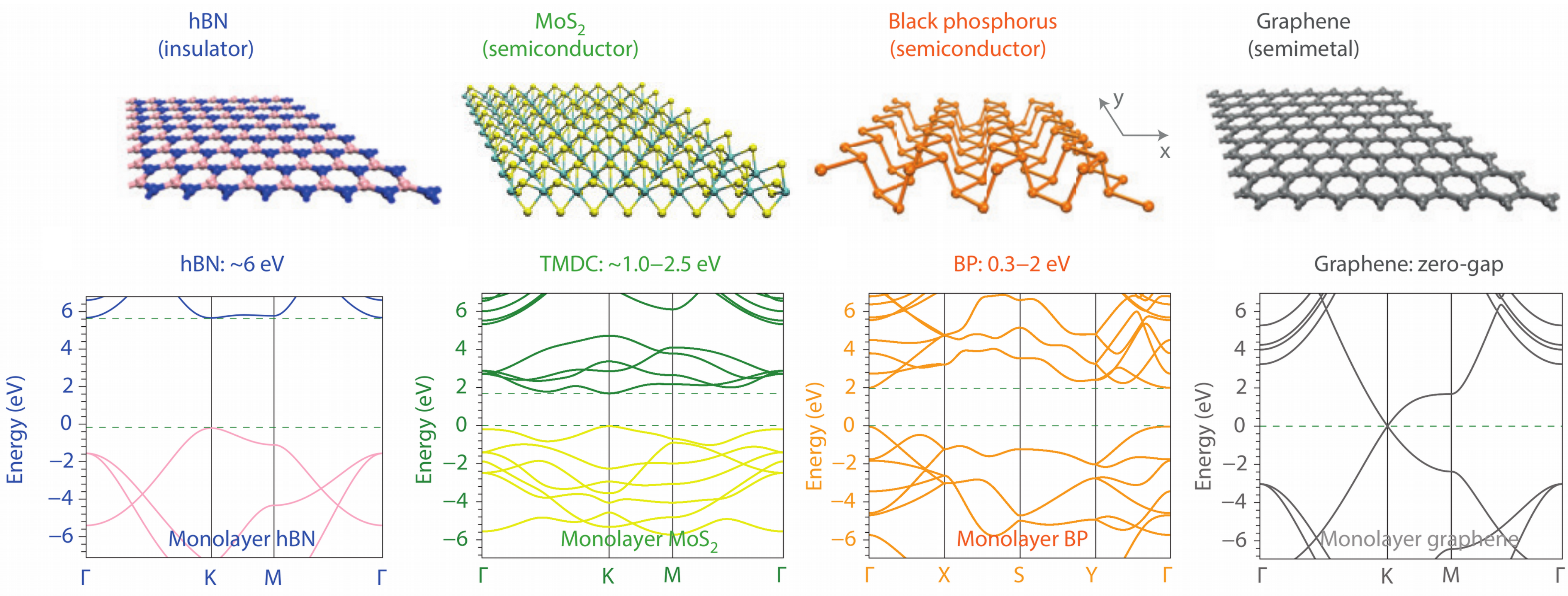




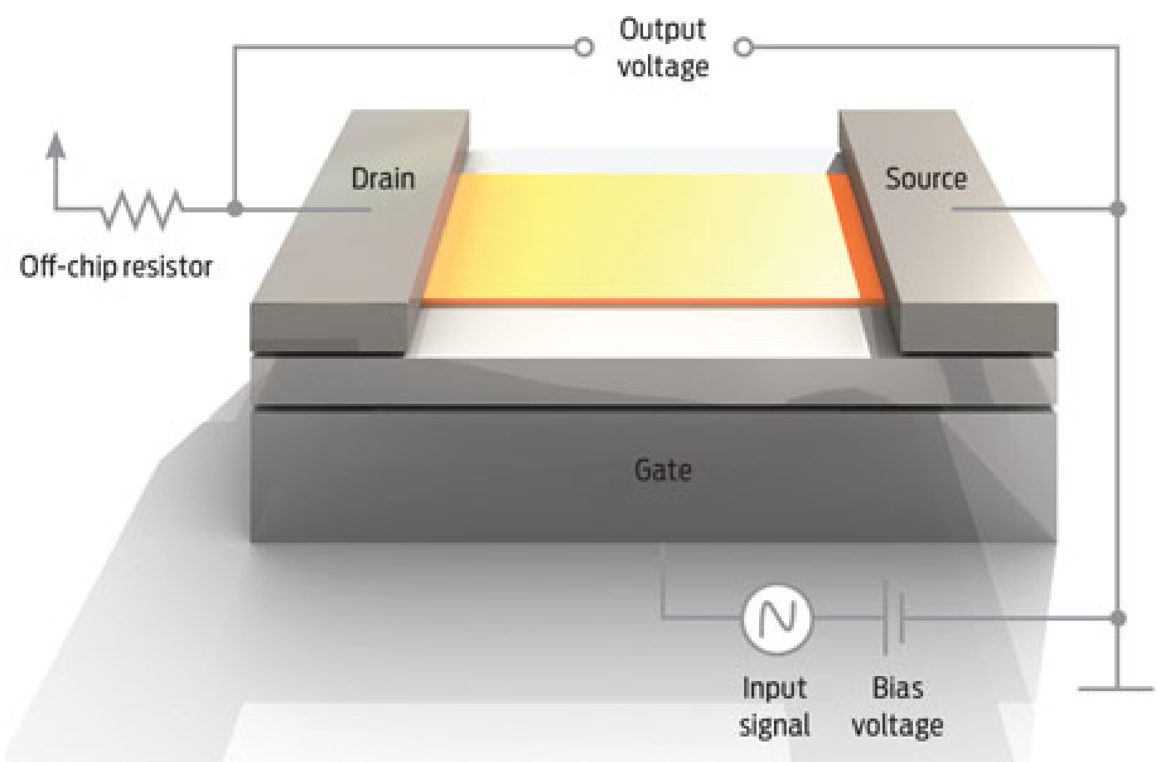
Objetivos

- Estructura de bandas
- DOS
- Funciones de Green (KPM)
- Conductividad
- Conductancia

Cristales en 2D

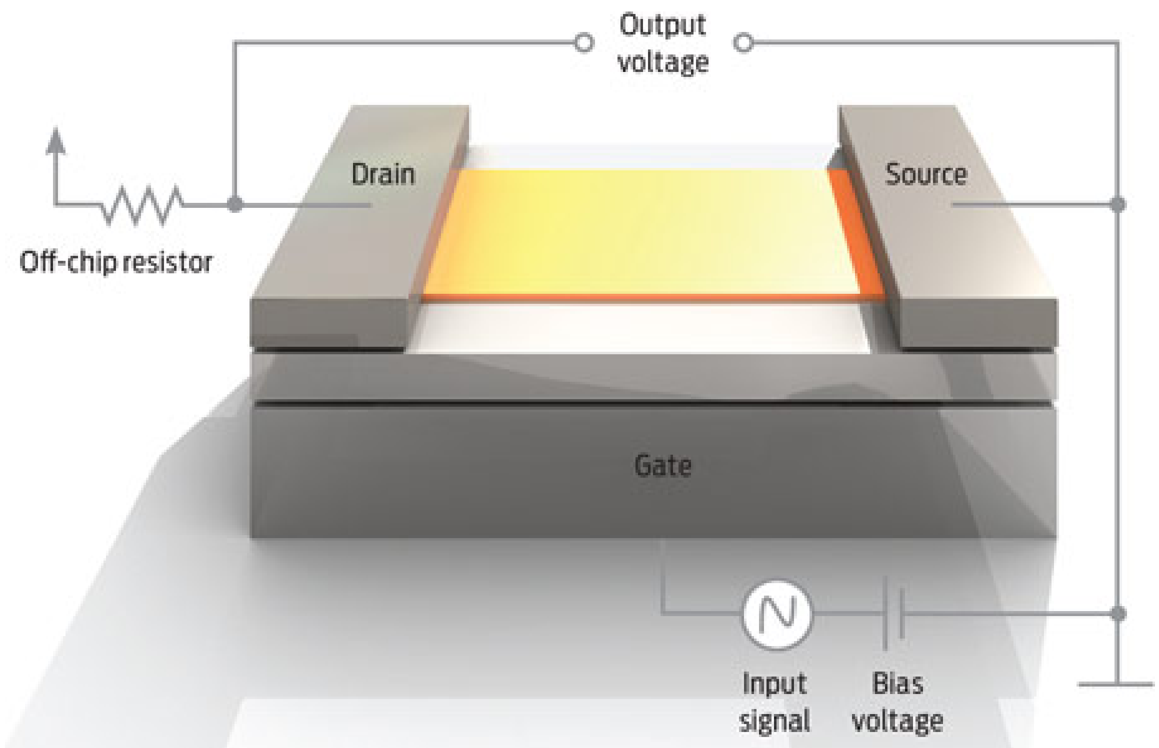


Transistor (FET – 2D)



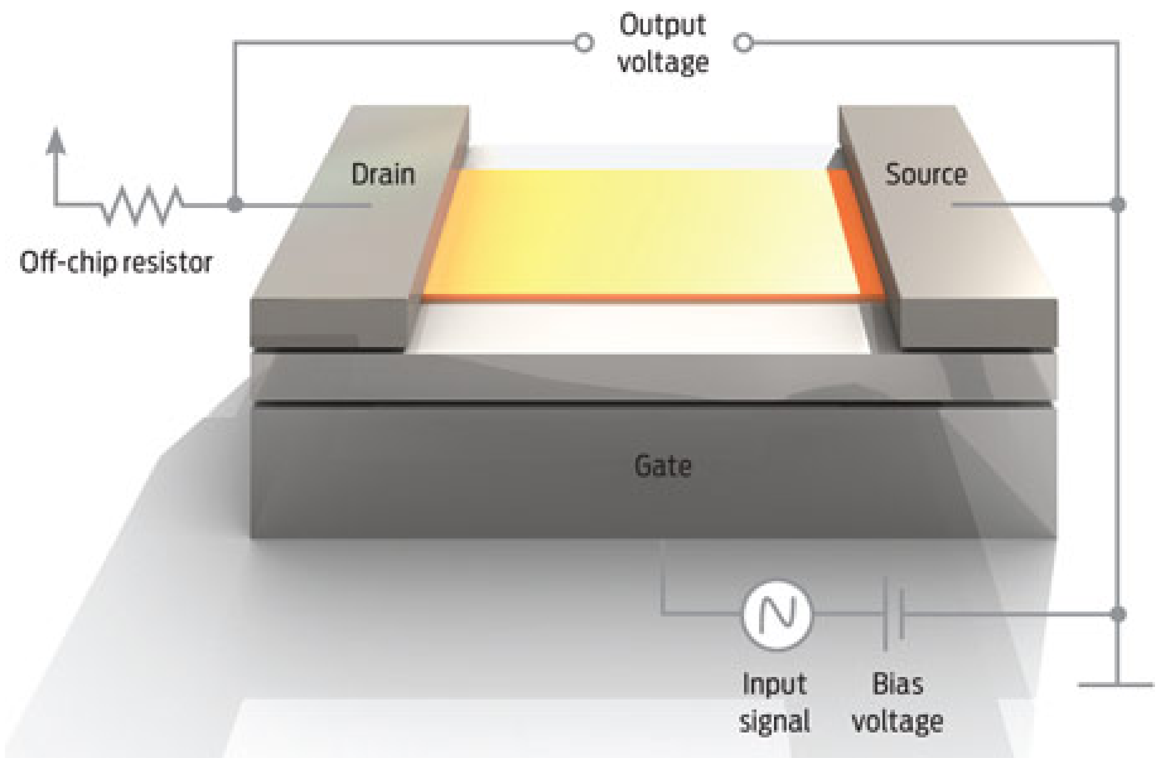
¿Por qué en 2D?

Transistor (FET – 2D)



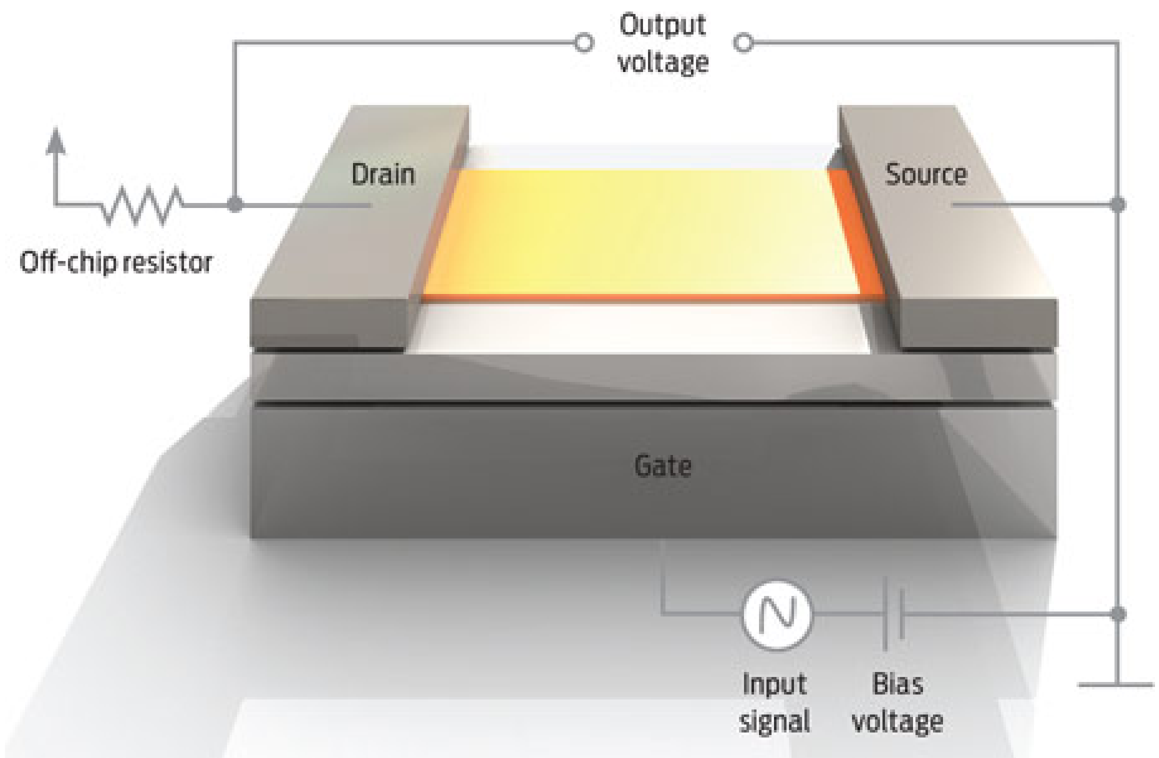
¿Por qué en 2D?
Tamaño y calentamiento

Transistor (FET – 2D)



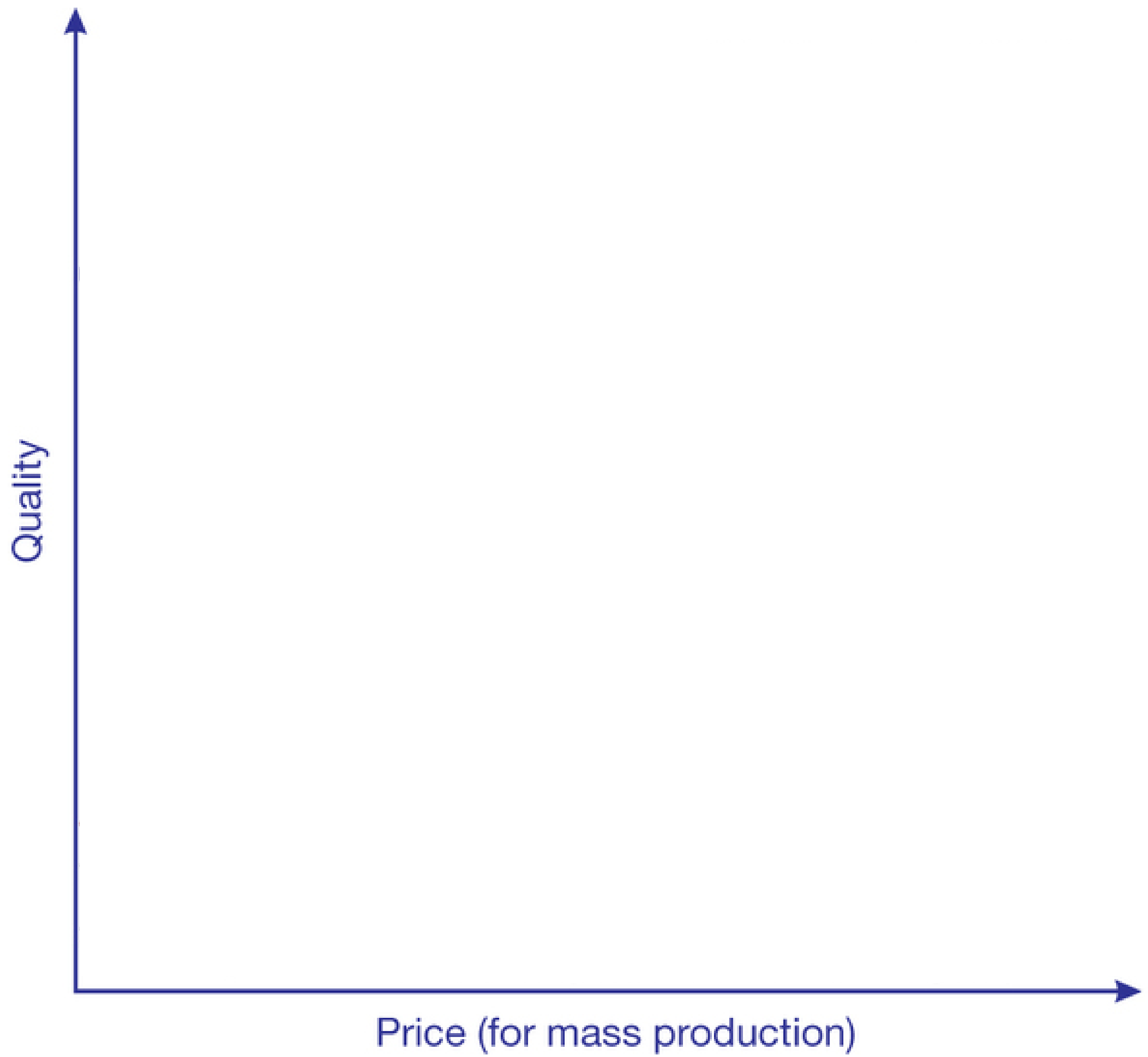
Propiedades (de bulto) del canal

Transistor (FET – 2D)



- Movilidad μ
- Conductividad de la hoja σ_{S}
- Densidad de portadores de carga n

Síntesis (grafeno)



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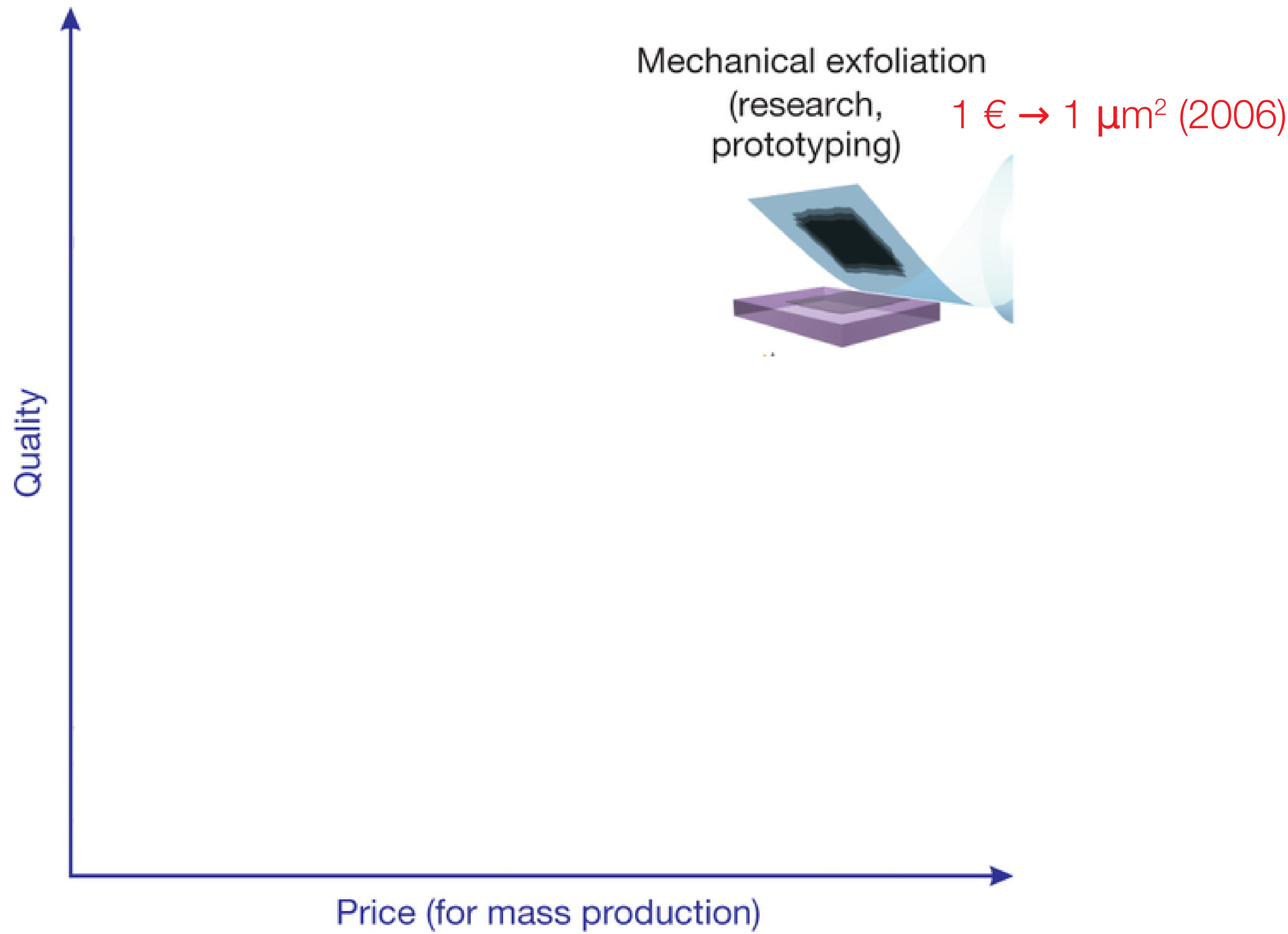

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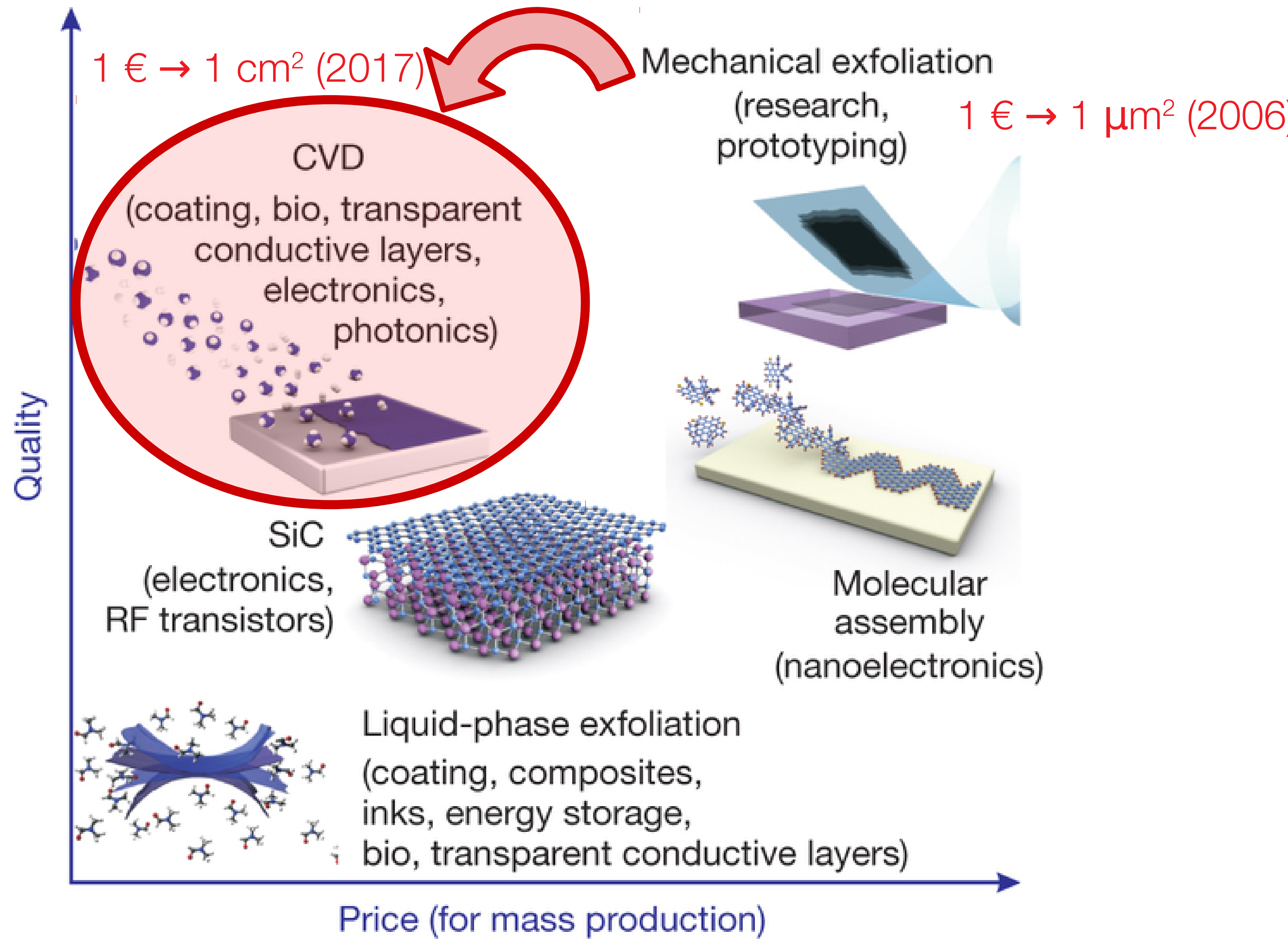
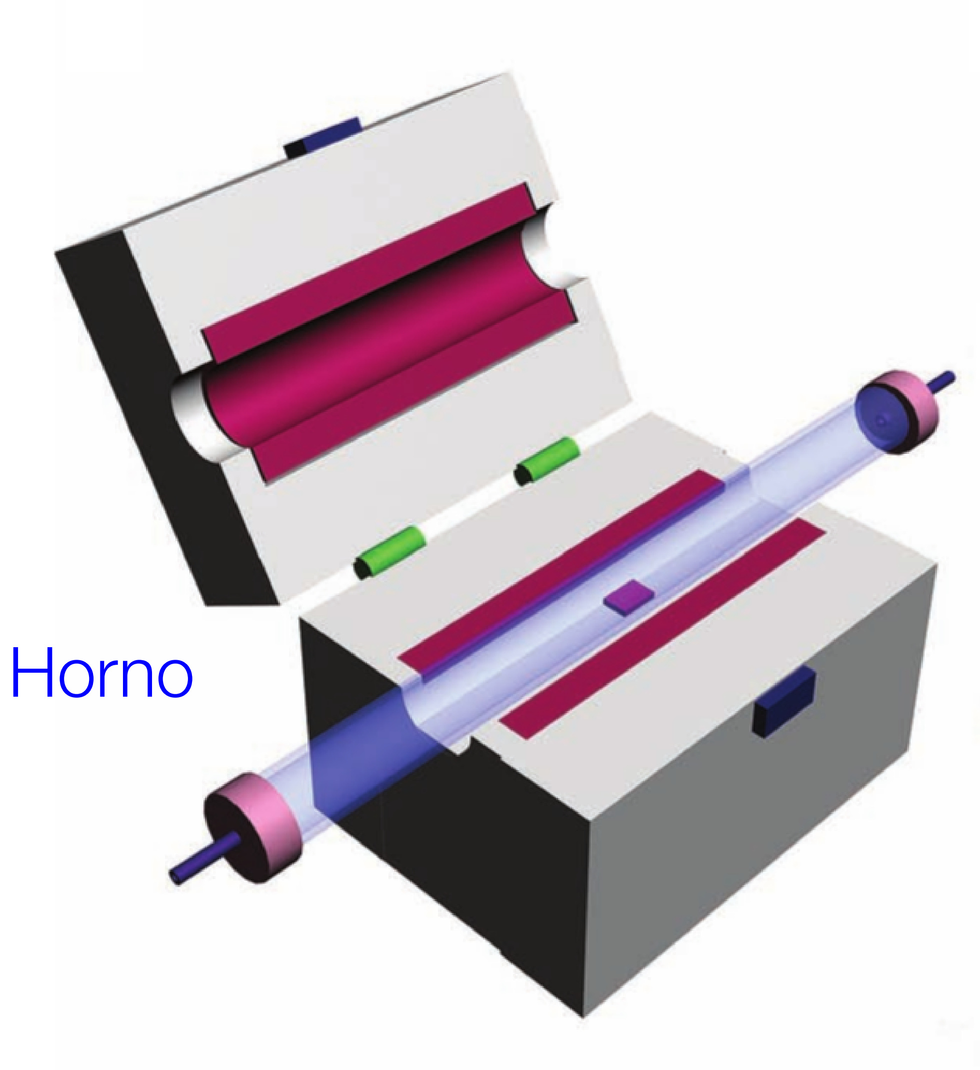
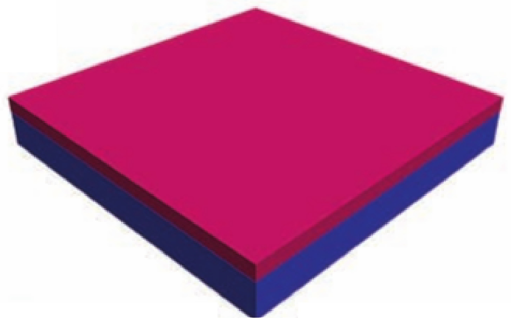


CVD (deposición química de vapor)





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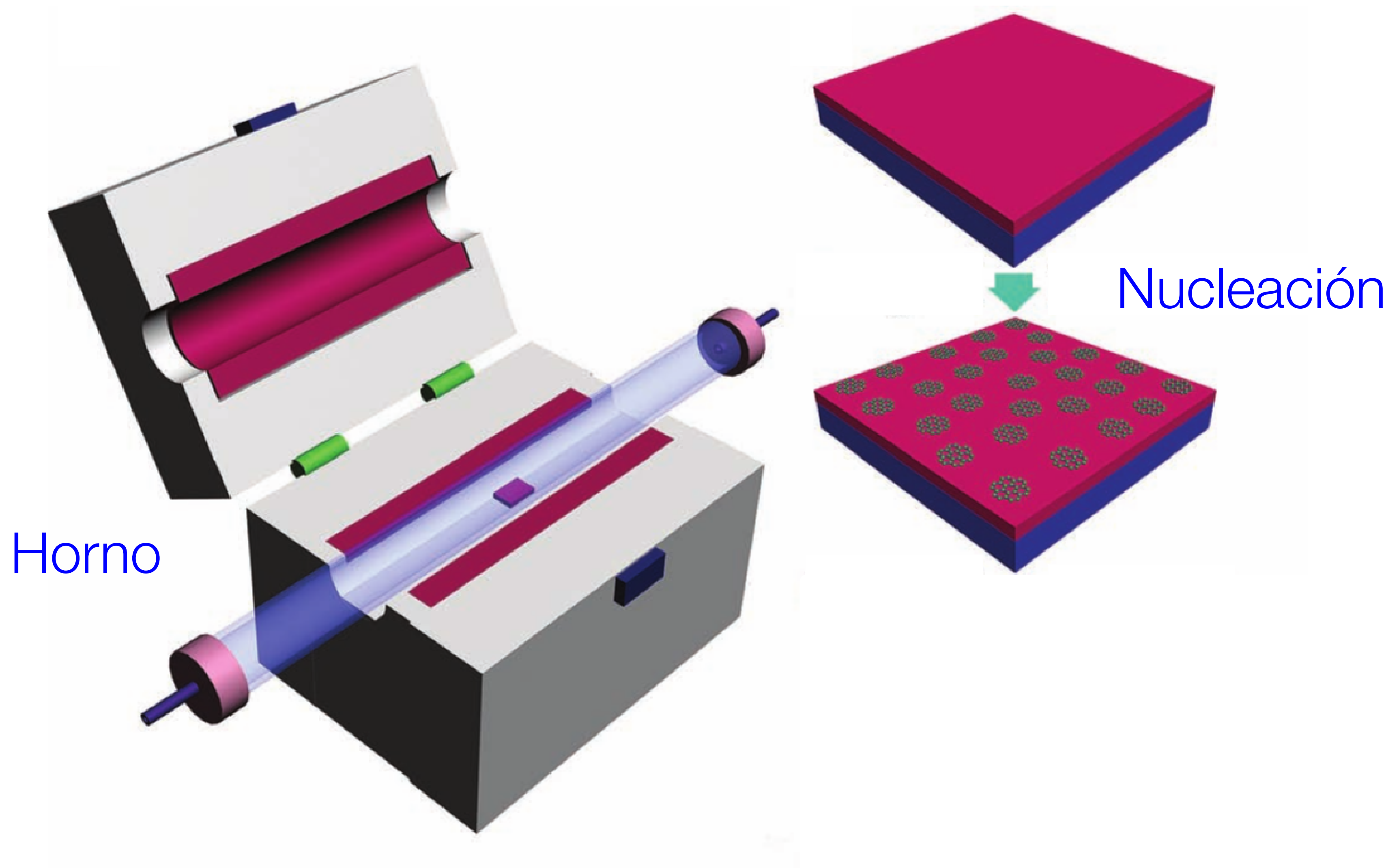

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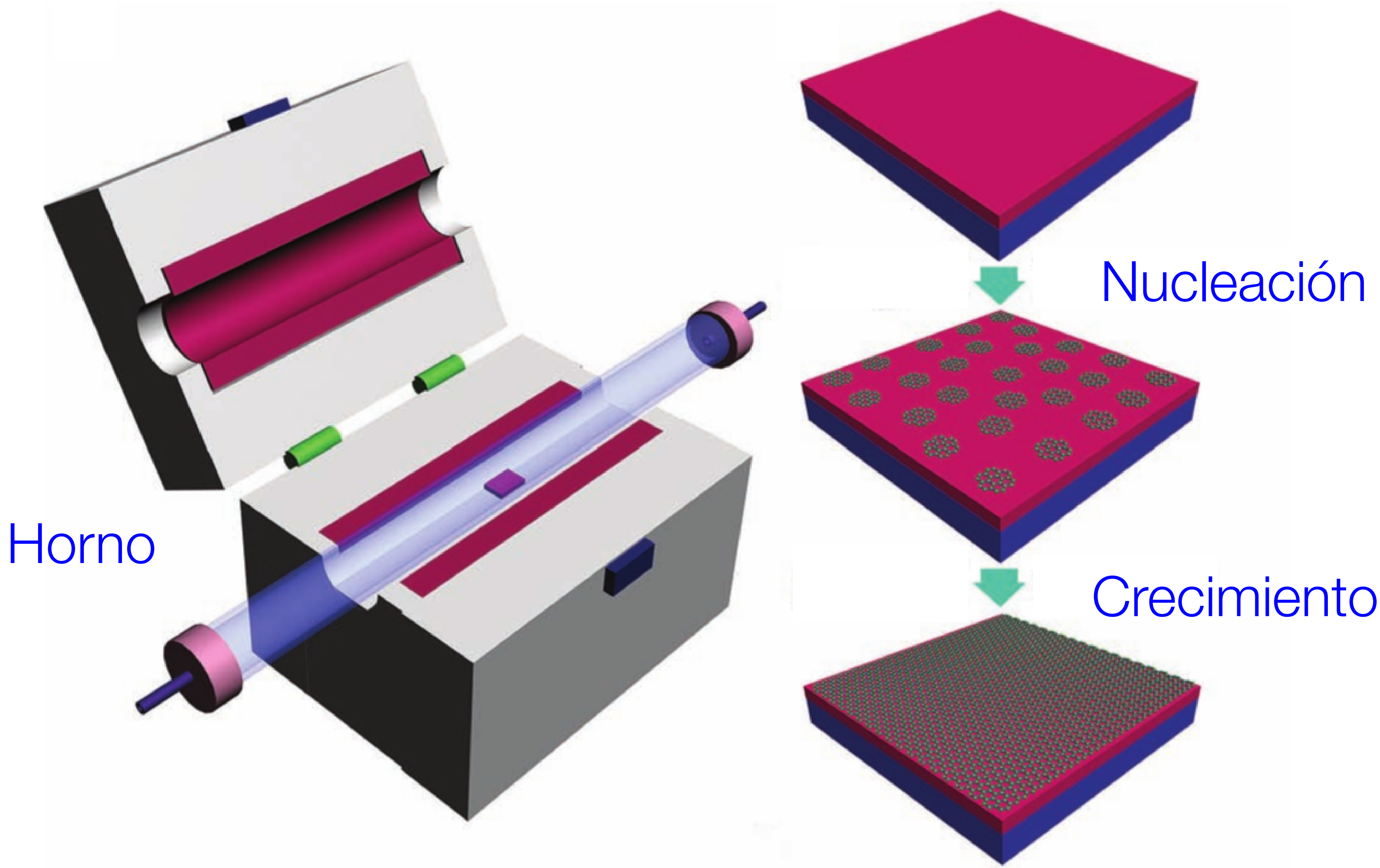
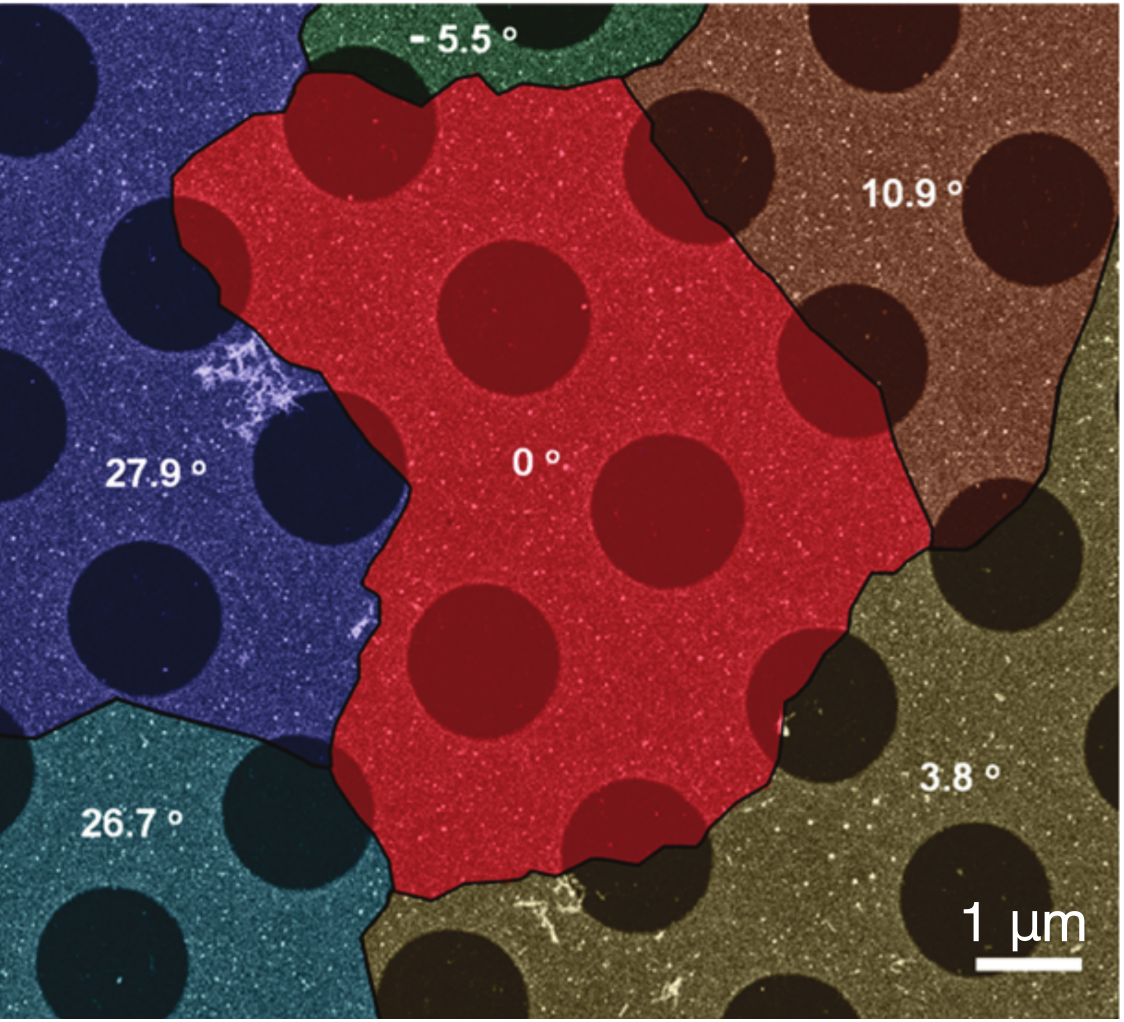


Grafeno CVD – policristalino



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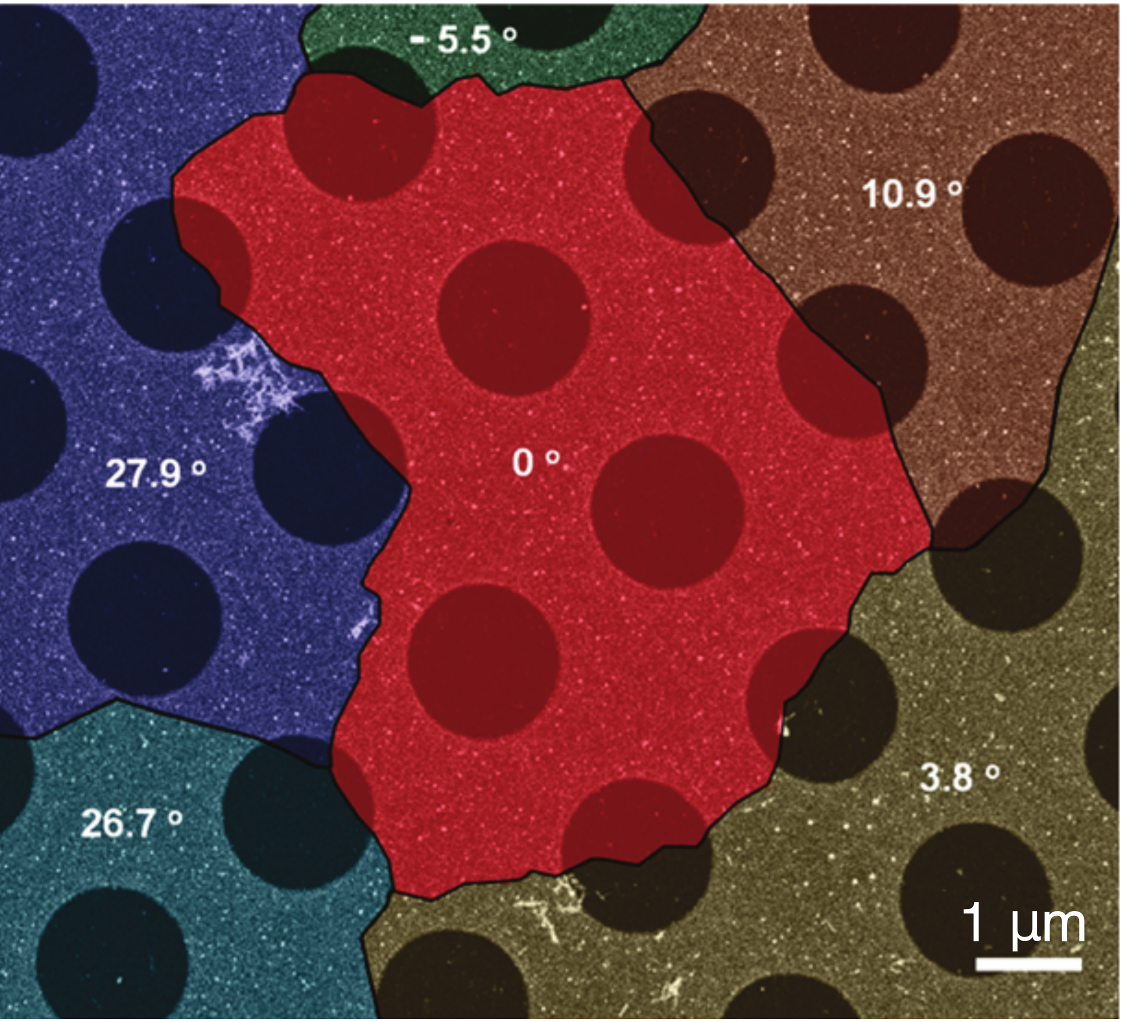

1 µm^2 → 40 millones de átomos

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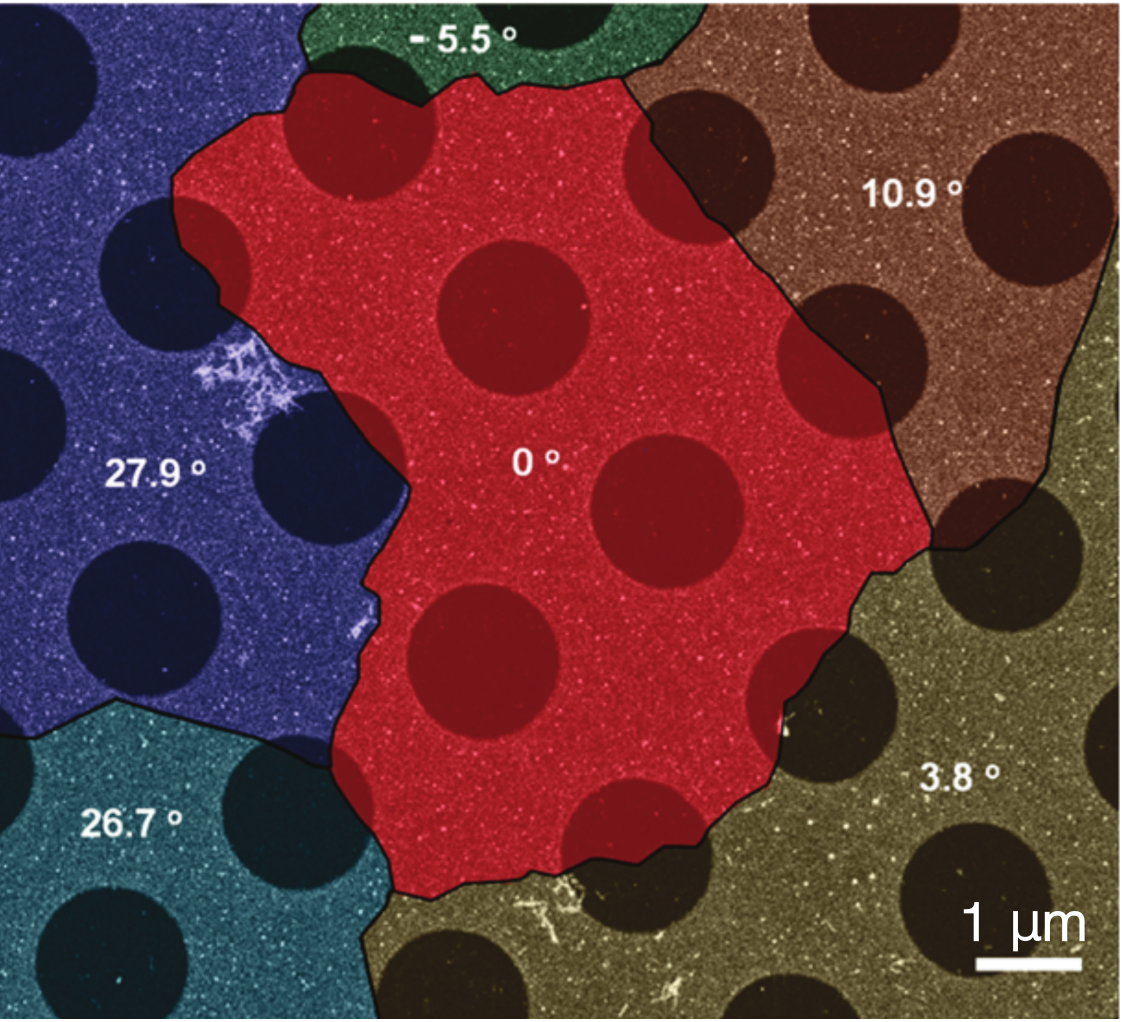

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(1) Red policristalina

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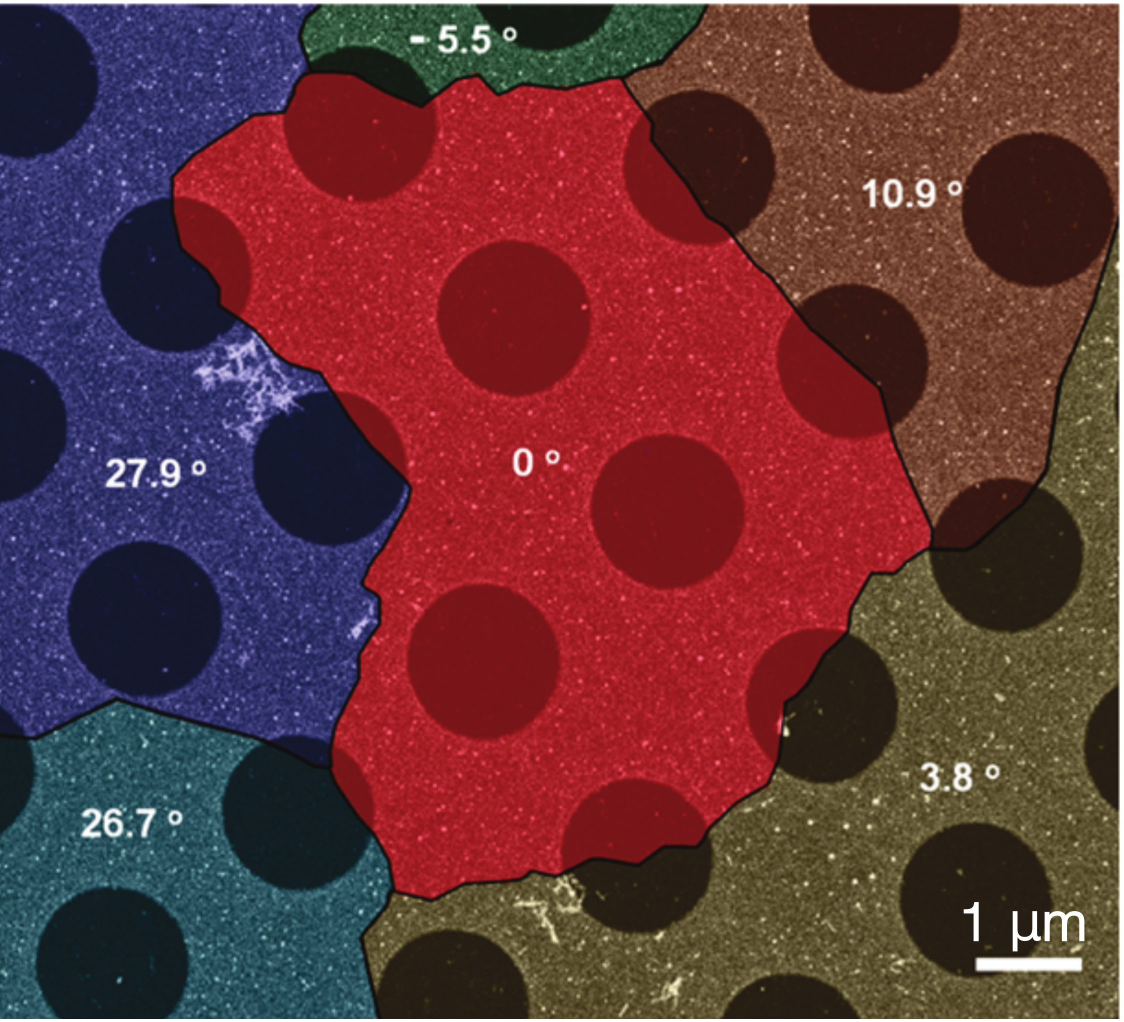

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(1) Red policristalina

(2) Hamiltoniano semiempírico

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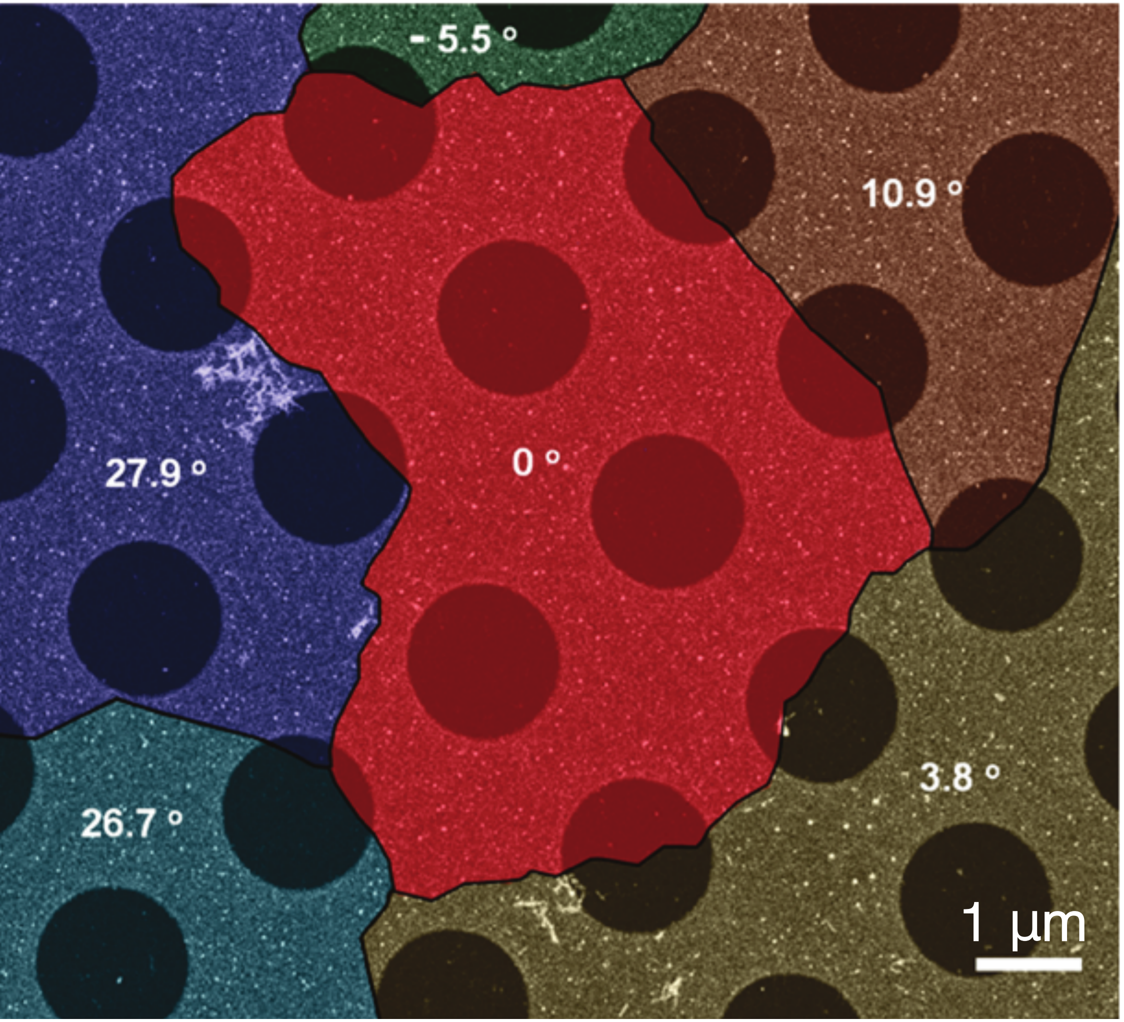


1 µm^2 → 40 millones de átomos

(1) Red policristalina

(2) Hamiltoniano semiempírico

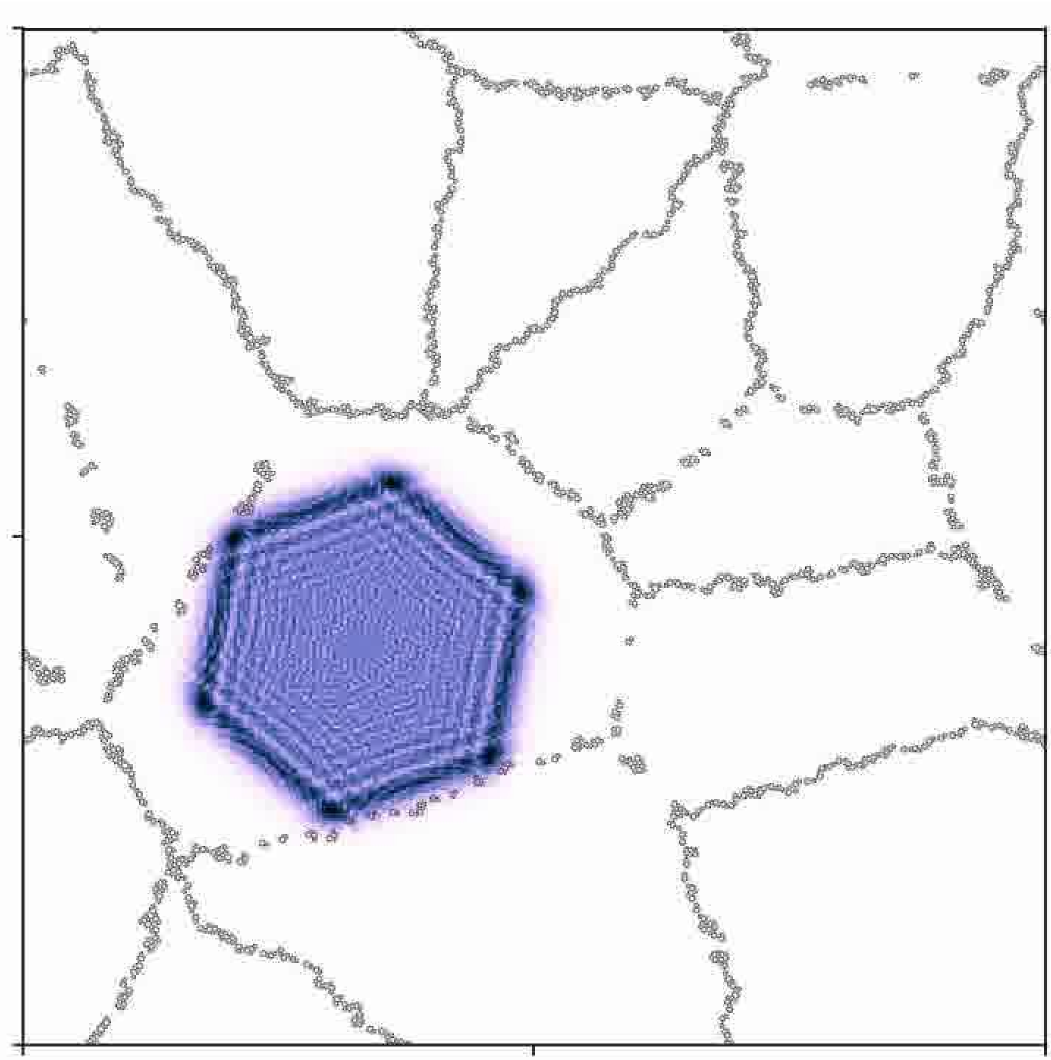
(3) Modelo de respuesta lineal

[Fórmula de Kubo-Greenwood]

Dinámica del paquete de onda

[Video]

Dinámica del paquete de onda



Curso

Hamiltoniano (approx.)

‘Toy model’

The shard

Grafeno (Hamiltoniano de amarre fuerte)

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OBJETIVO (approx.):

- Modelar electrones en un cristal para calcular al estructura de bandas electrónicas.

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Es un método semiempírico

LCAO- Combinación lineal de orbitales atómicos
(Método de Hückel)

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Es un método semiempírico

LCAO- Combinación lineal de orbitales atómicos
(Método de Hückel)

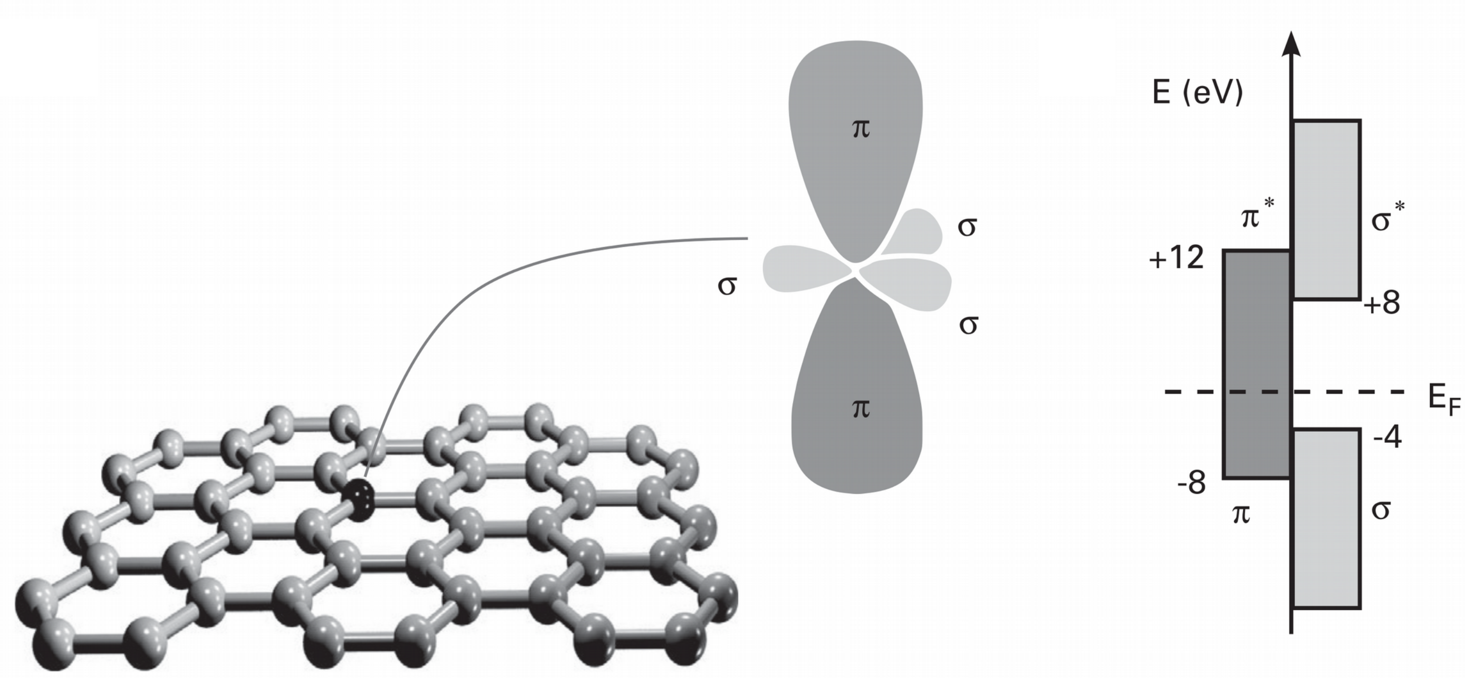
Ventajas:

- Permite realizar cálculos de manera veloz en sistemas *MUY GRANDES*

Desventajas:

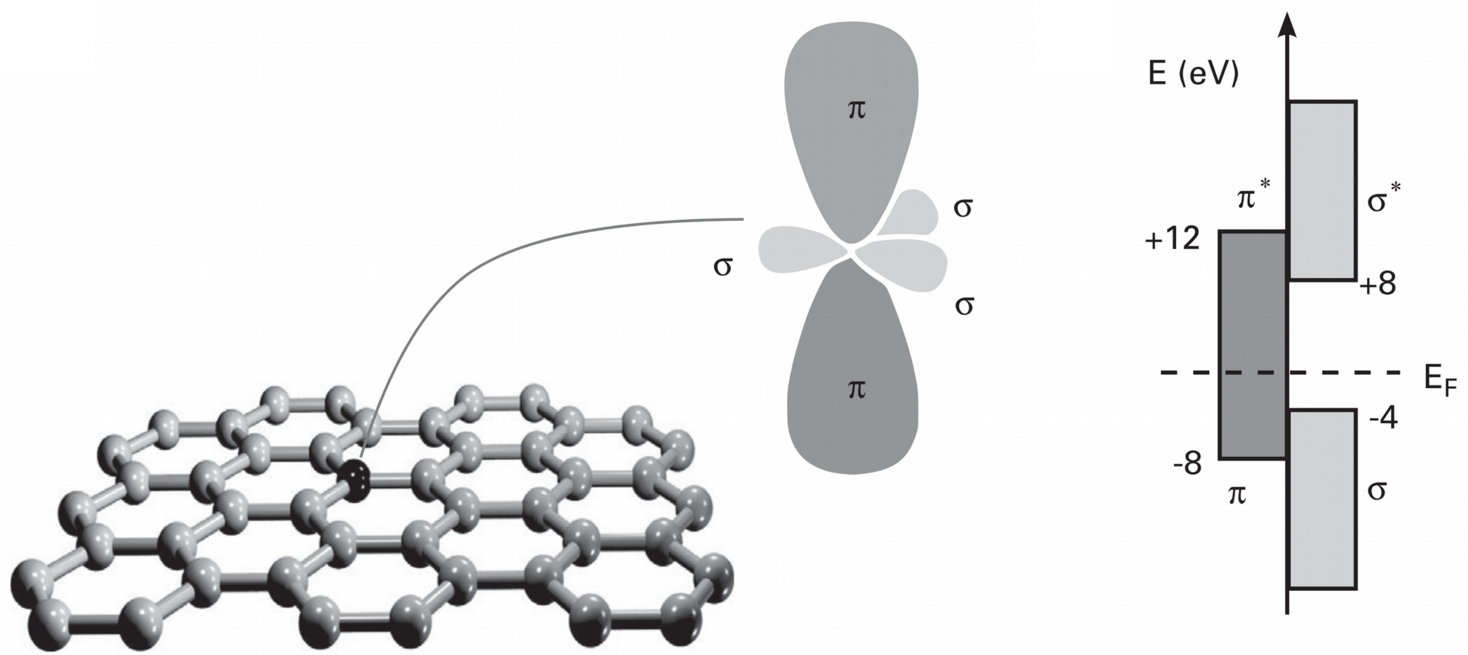
- *IGNORA LA INTERACCION* e-e

Grafeno (Hamiltoniano de amarre fuerte)



$$\mathcal{H} = -t \sum_{\langle \boldsymbol{i},\boldsymbol{j} \rangle} |\boldsymbol{i}\rangle\langle \boldsymbol{j}| + \text{h.c.}$$

Grafeno (Hamiltoniano de amarre fuerte)



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Idea básica: Conectividad (lattice) → Hamiltoniano

Grafeno (Hamiltoniano de amarre fuerte)

En cada célda unitaria:

$$\psi_{\rm uc}(\mathbf{r}) = a\, p_z(\mathbf{r} - \mathbf{r}_A) + b\, p_z(\mathbf{r} - \mathbf{r}_B)$$

Teorema de Bloch las eigenfunciones evaluadas en dos puntos de la red de Bravais $\mathbf{R}_i$ and $\mathbf{R}_j$ difieren sólo por un factor $\exp(i\mathbf{k} \cdot (\mathbf{R}_i - \mathbf{R}_j))$

$$\Psi(\mathbf{k}, \mathbf{r}) = c_A(\mathbf{k})\tilde{p}_z^A(\mathbf{k}, \mathbf{r}) + c_B(\mathbf{k})\tilde{p}_z^B(\mathbf{k}, \mathbf{r}),$$

$$\tilde{p}_z^A(\mathbf{k}, \mathbf{r}) = \frac{1}{\sqrt{N_{\rm cells}}} \sum_j \mathrm{e}^{\mathbf{ik.R}_j} p_z(\mathbf{r} - \mathbf{r}_A - \mathbf{R}_j),$$

$$\tilde{p}_z^B(\mathbf{k}, \mathbf{r}) = \frac{1}{\sqrt{N_{\rm cells}}} \sum_j \mathrm{e}^{\mathbf{ik.R}_j} p_z(\mathbf{r} - \mathbf{r}_B - \mathbf{R}_j),$$

Despreciamos el overlap

$$s = \langle p_z^A | p_z^B \rangle$$

Entonces la condición de ortogonalidad es: $\langle \tilde{p}_z^\alpha(\mathbf{k}) \mid \tilde{p}_z^\beta(\mathbf{k}')\rangle = \delta_{\mathbf{k},\mathbf{k}'}\delta_{\alpha,\beta},$

Grafeno (Hamiltoniano de amarre fuerte)

Usando la ortogonalidad previa en la ecuación de Scroedinger

$$\begin{pmatrix} \mathcal{H}_{AA}(\mathbf{k}) & \mathcal{H}_{AB}(\mathbf{k}) \\ \mathcal{H}_{BA}(\mathbf{k}) & \mathcal{H}_{BB}(\mathbf{k}) \end{pmatrix} \begin{pmatrix} c_A(\mathbf{k}) \\ c_B(\mathbf{k}) \end{pmatrix} = E(\mathbf{k}) \begin{pmatrix} c_A(\mathbf{k}) \\ c_B(\mathbf{k}) \end{pmatrix}$$

$$\mathcal{H}_{AA}(\mathbf{k}) = \frac{1}{N_{\text{cells}}} \sum_{i,j} \mathrm{e}^{\mathrm{i}\mathbf{k}.(\mathbf{R}_j - \mathbf{R}_i)} \langle p_z^{A,\mathbf{R}_i} \mid \mathcal{H} \mid p_z^{A,\mathbf{R}_j} \rangle,$$

Referencia de energía

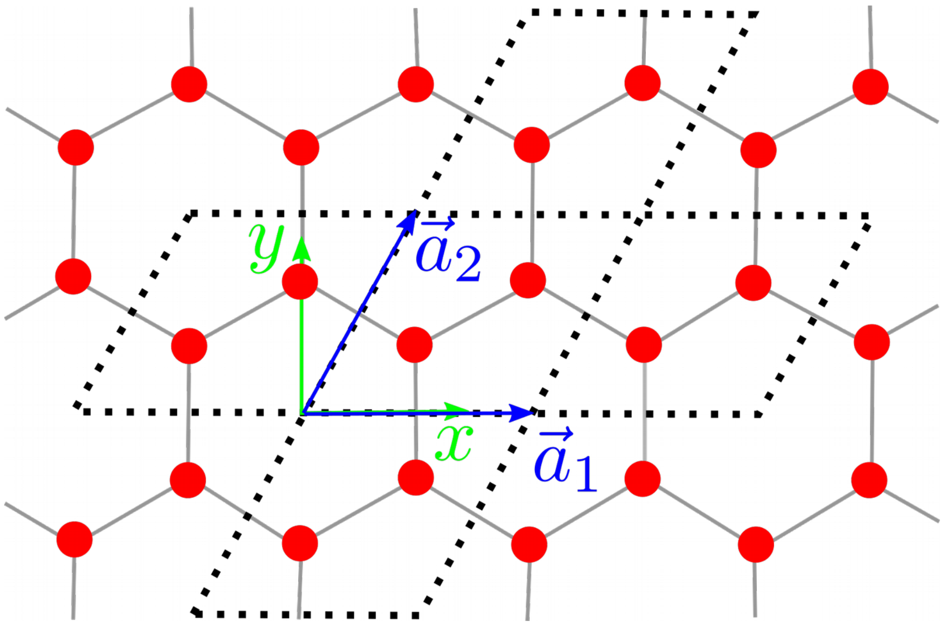
$$\mathcal{H}_{AB}(\mathbf{k}) = \frac{1}{N_{\text{cells}}} \sum_{i,j} \mathrm{e}^{\mathrm{i}\mathbf{k}.(\mathbf{R}_j - \mathbf{R}_i)} \langle p_z^{A,\mathbf{R}_i} \mid \mathcal{H} \mid p_z^{B,\mathbf{R}_j} \rangle,$$

$$\begin{aligned} \mathcal{H}_{AB}(\mathbf{k}) &= \langle p_z^{A,0} | \mathcal{H} | p_z^{B,0} \rangle + \mathrm{e}^{-\mathrm{i}\mathbf{k}.\mathbf{a}_1} \langle p_z^{A,0} | \mathcal{H} | p_z^{B,-\mathbf{a}_1} \rangle + \mathrm{e}^{-\mathrm{i}\mathbf{k}.\mathbf{a}_2} \langle p_z^{A,0} | \mathcal{H} | p_z^{B,-\mathbf{a}_2} \rangle \\ &= -\gamma_0 \alpha(\mathbf{k}), \end{aligned}$$

$$\alpha(\mathbf{k}) = (1 + \mathrm{e}^{-\mathrm{i}\mathbf{k}.\mathbf{a}_1} + \mathrm{e}^{-\mathrm{i}\mathbf{k}.\mathbf{a}_2}).$$

$$\mathcal{H}(\mathbf{k}) = \begin{pmatrix} 0 & -\gamma_0 \alpha(\mathbf{k}) \\ -\gamma_0 \alpha(\mathbf{k})^* & 0 \end{pmatrix}$$

Celda unitaria → 1 zona de Brillouin



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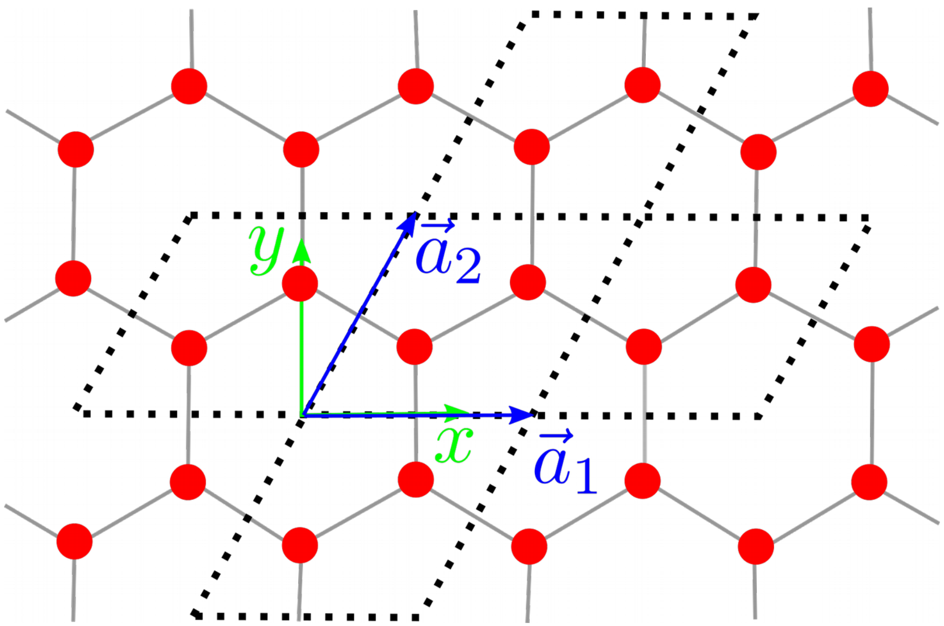

$$\begin{bmatrix} a_{1x} & a_{2x} \\ a_{1y} & a_{2y} \end{bmatrix} \begin{bmatrix} b_{1x} & b_{2x} \\ b_{1y} & b_{2y} \end{bmatrix} = \begin{bmatrix} 2\pi & 0 \\ 0 & 2\pi \end{bmatrix}$$

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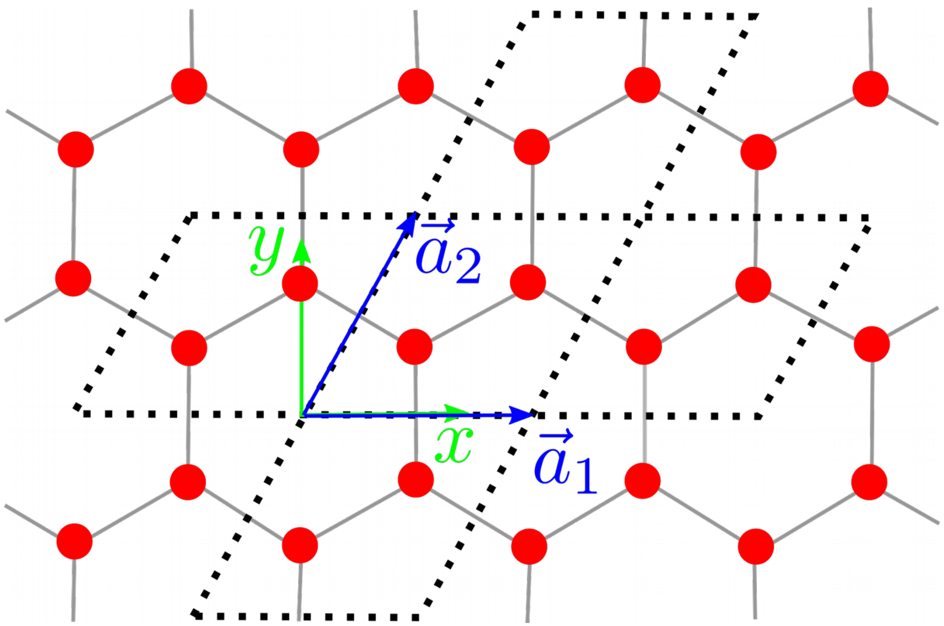

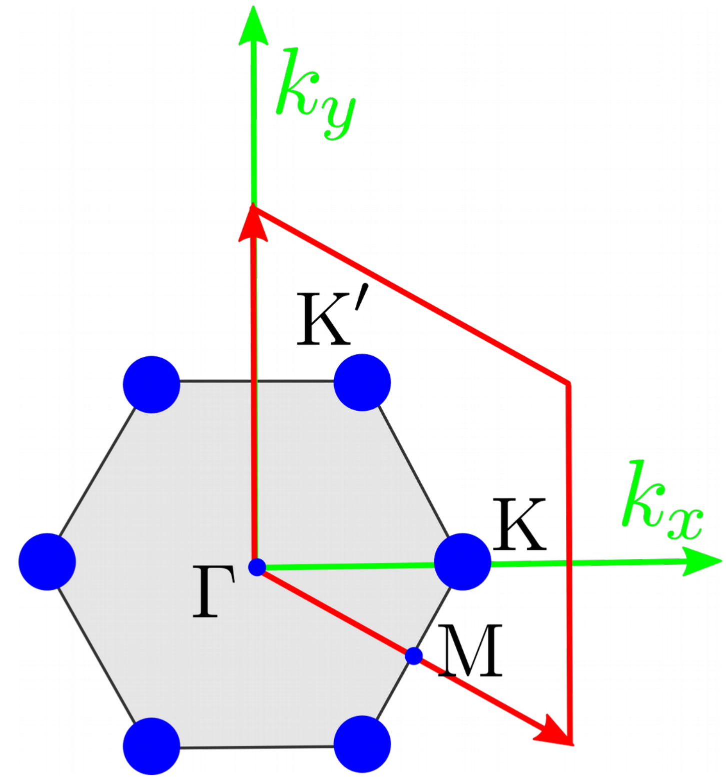

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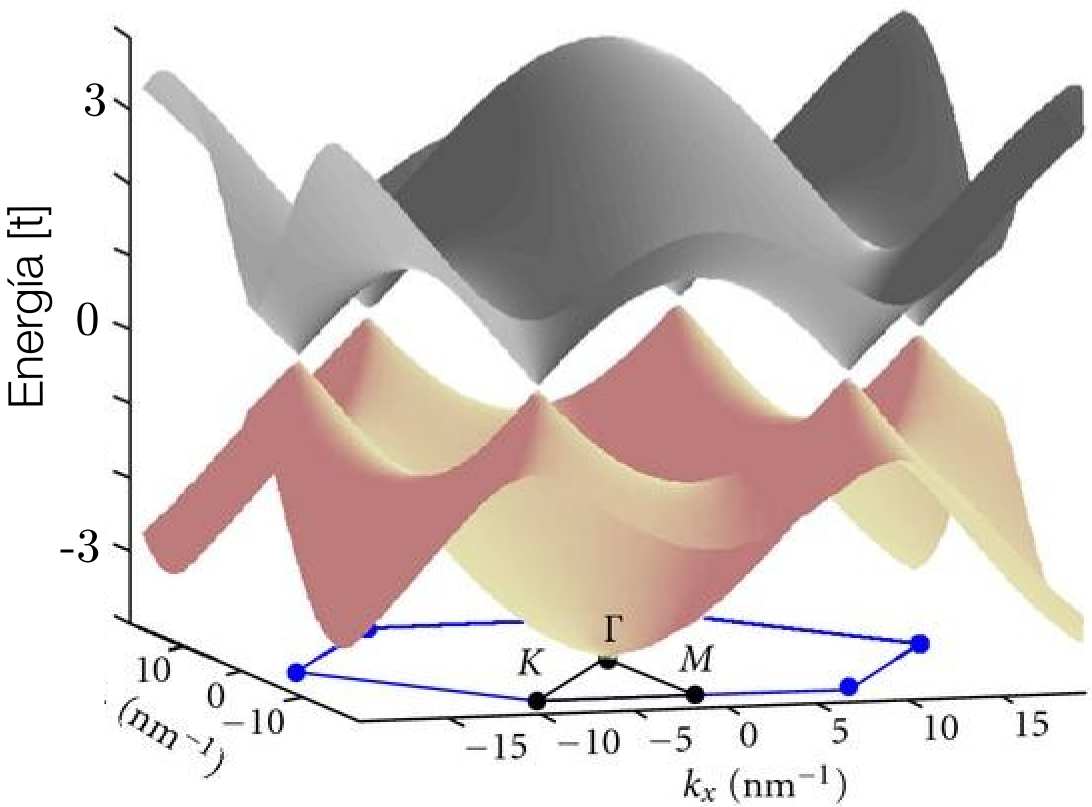
$$H(\vec{k}) = \begin{bmatrix} 0 & -t(1+\mathrm{e}^{-i\vec{k}\cdot\vec{a}_1}+\mathrm{e}^{-i\vec{k}\cdot\vec{a}_2}) \\ -t(1+\mathrm{e}^{i\vec{k}\cdot\vec{a}_1}+\mathrm{e}^{i\vec{k}\cdot\vec{a}_2}) & 0 \end{bmatrix}$$



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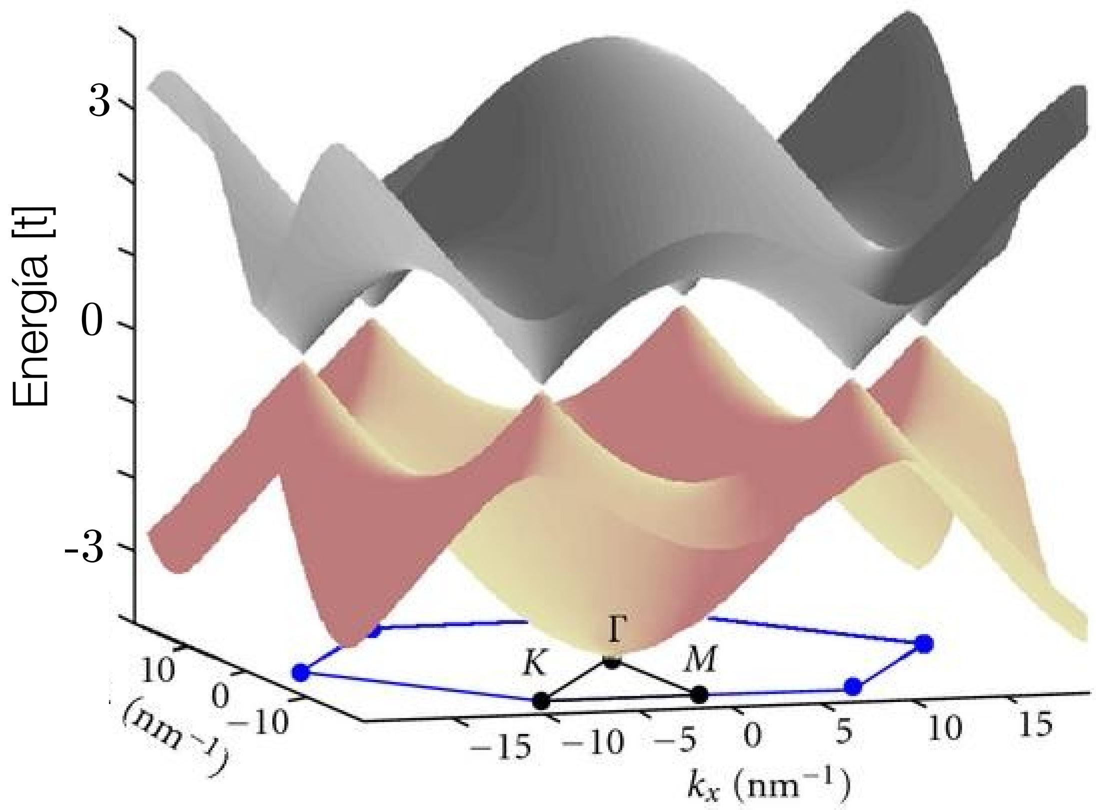
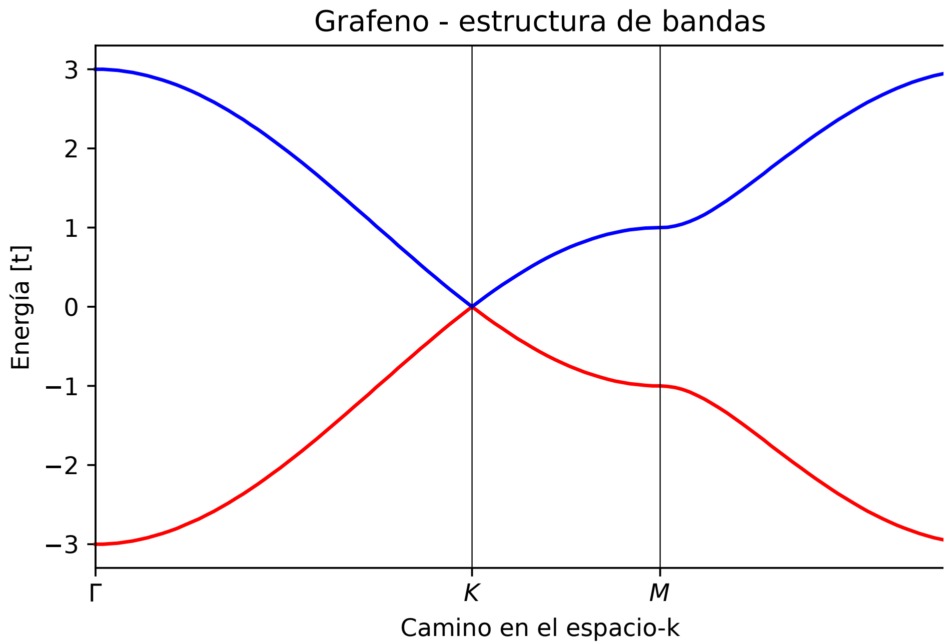
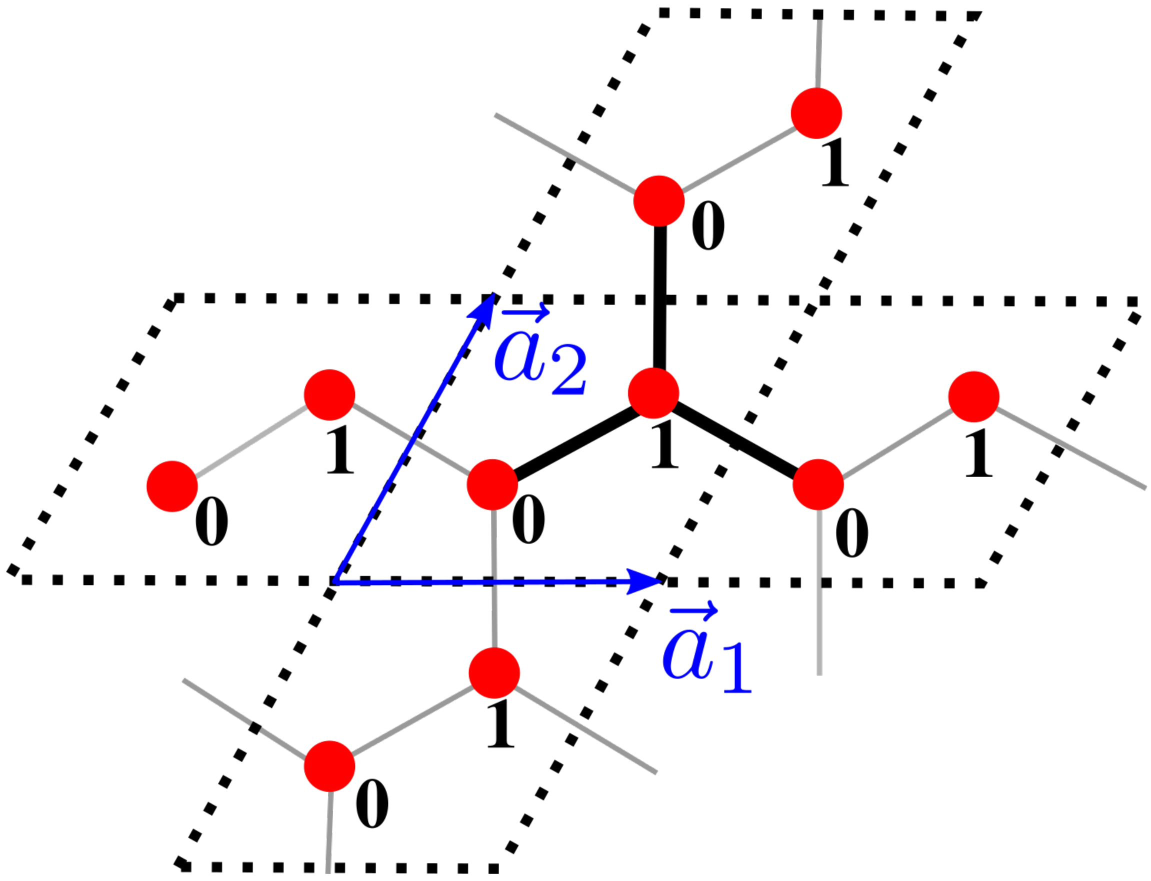




pythtb

Sinisa Coh (University of California at Riverside) and David Vanderbilt (Rutgers University)



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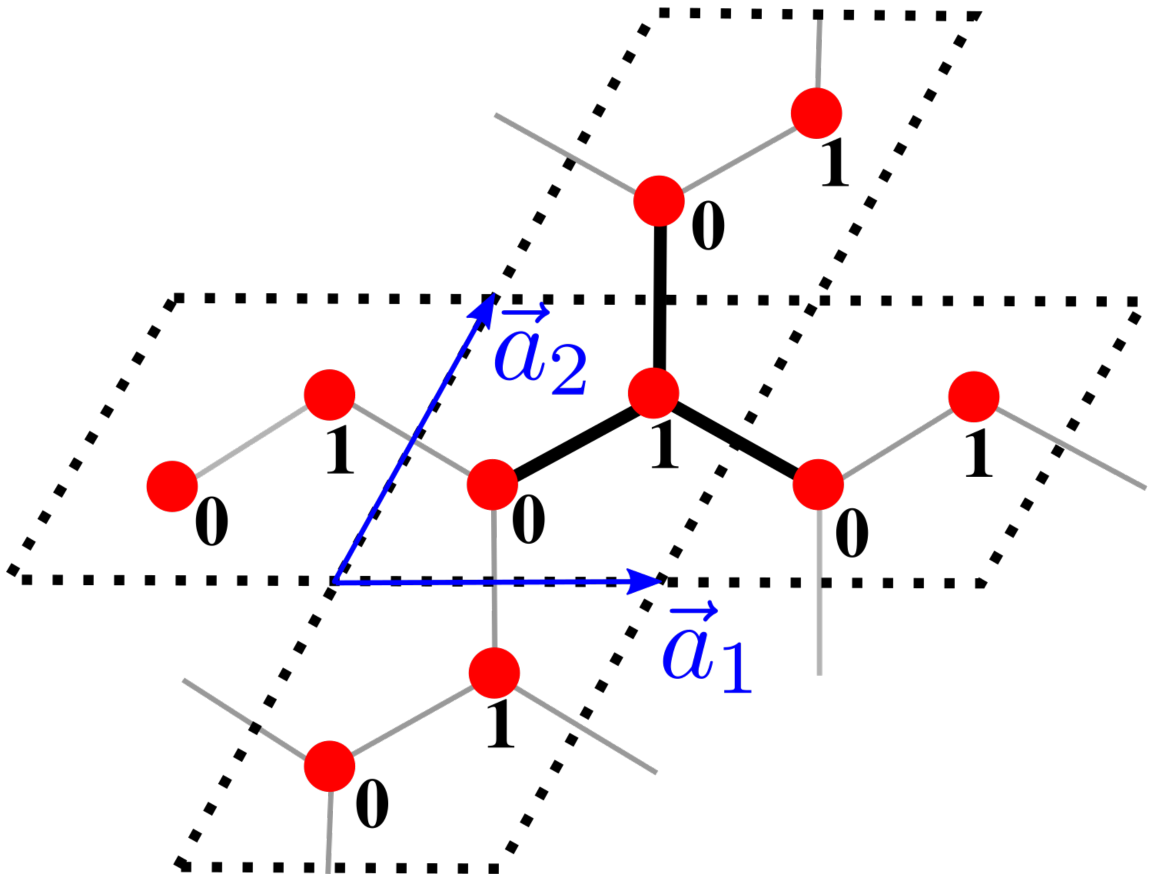


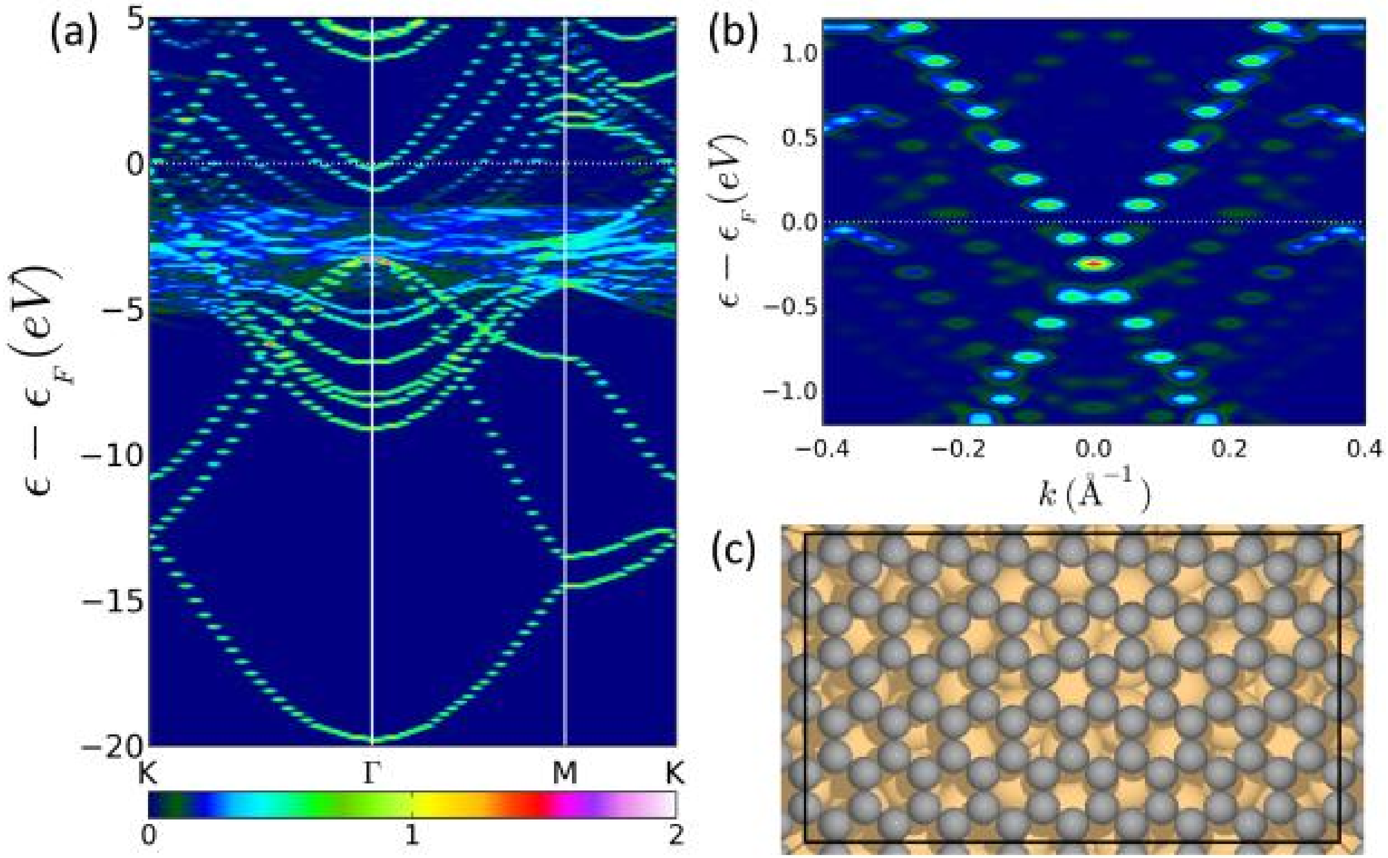
Estructura de bandas

Superceldas

Ribbons

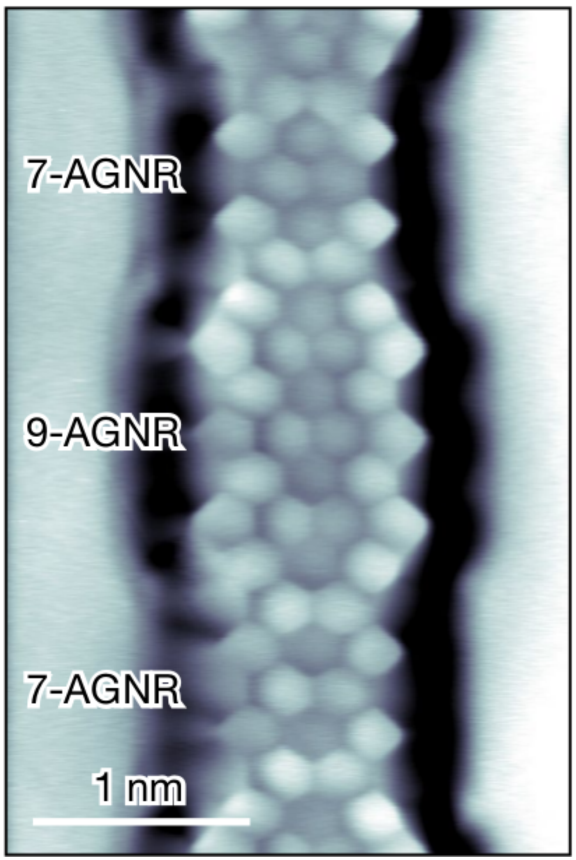
DOS

Unfold brillouin zone (Graphene@Cu(111))

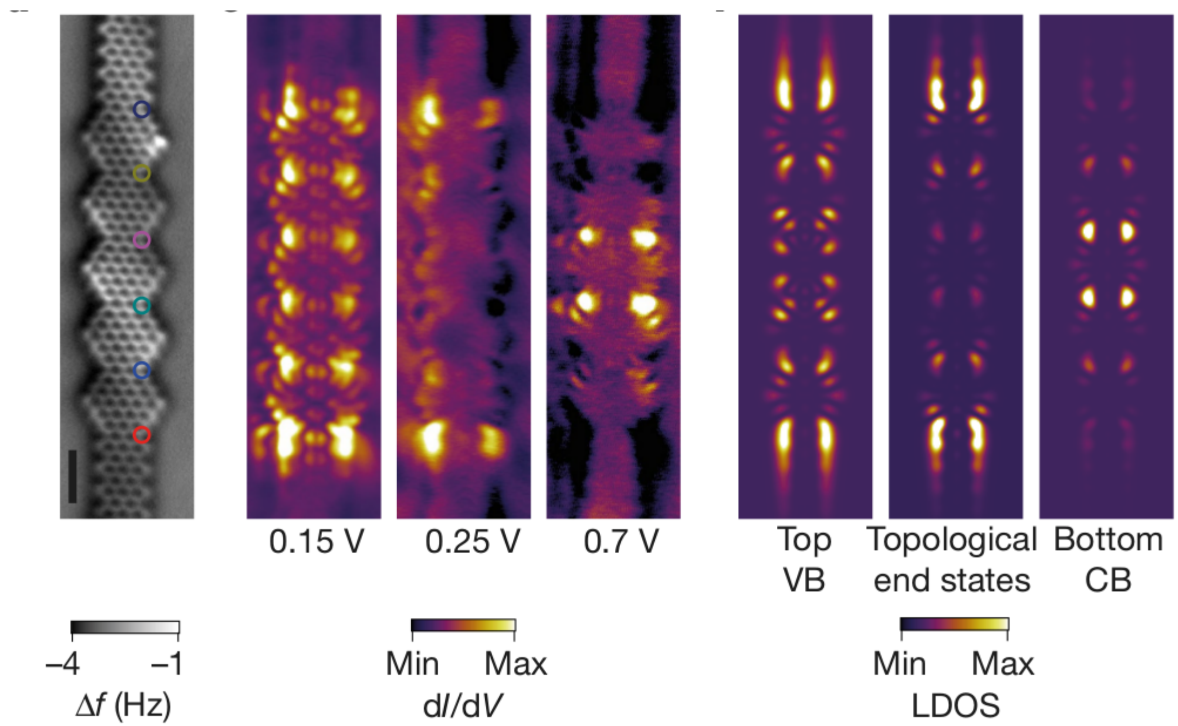


Nanoribbons

Topological band engineering of graphene nanoribbons
Nature **560**, 204-208 (2018)



Engineering of robust topological quantum phases in graphene nanoribbons
Nature **560**, 209-213 (2018)

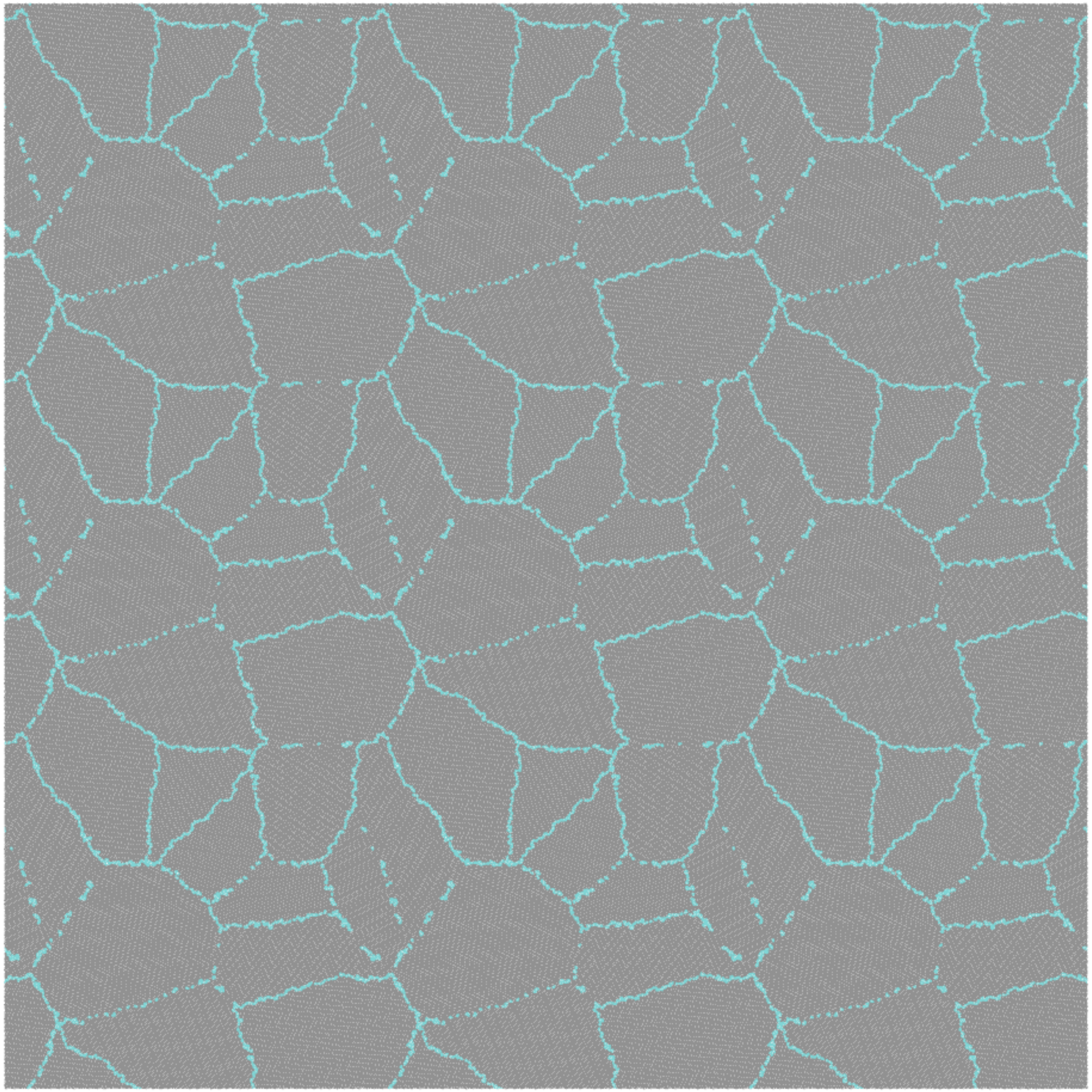


Operador evolución

[video]

Construir el Hamiltoniano

Amarre fuerte (Tight-binding) → Matriz de conectividad



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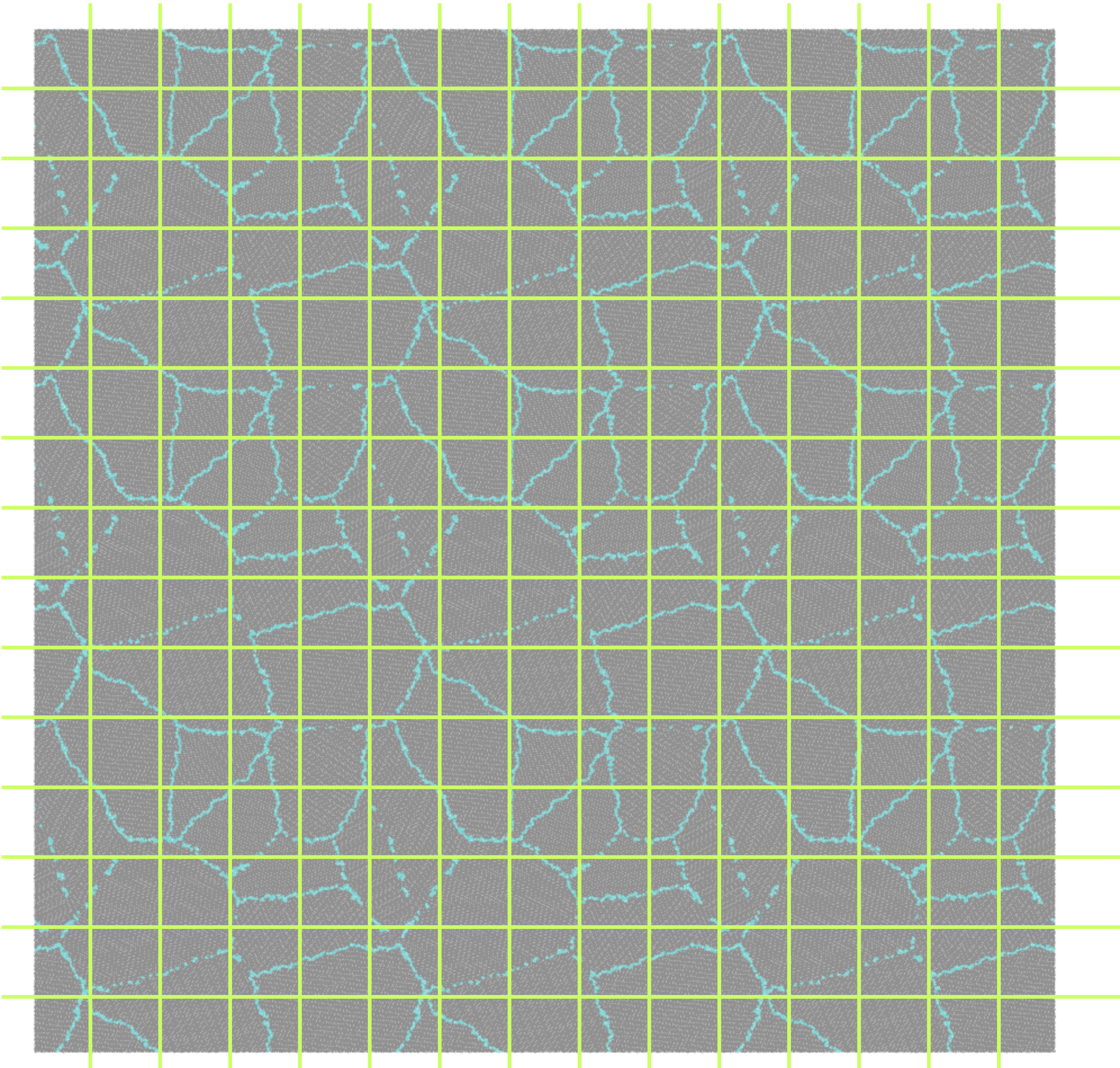

- Cells(i, j, #)

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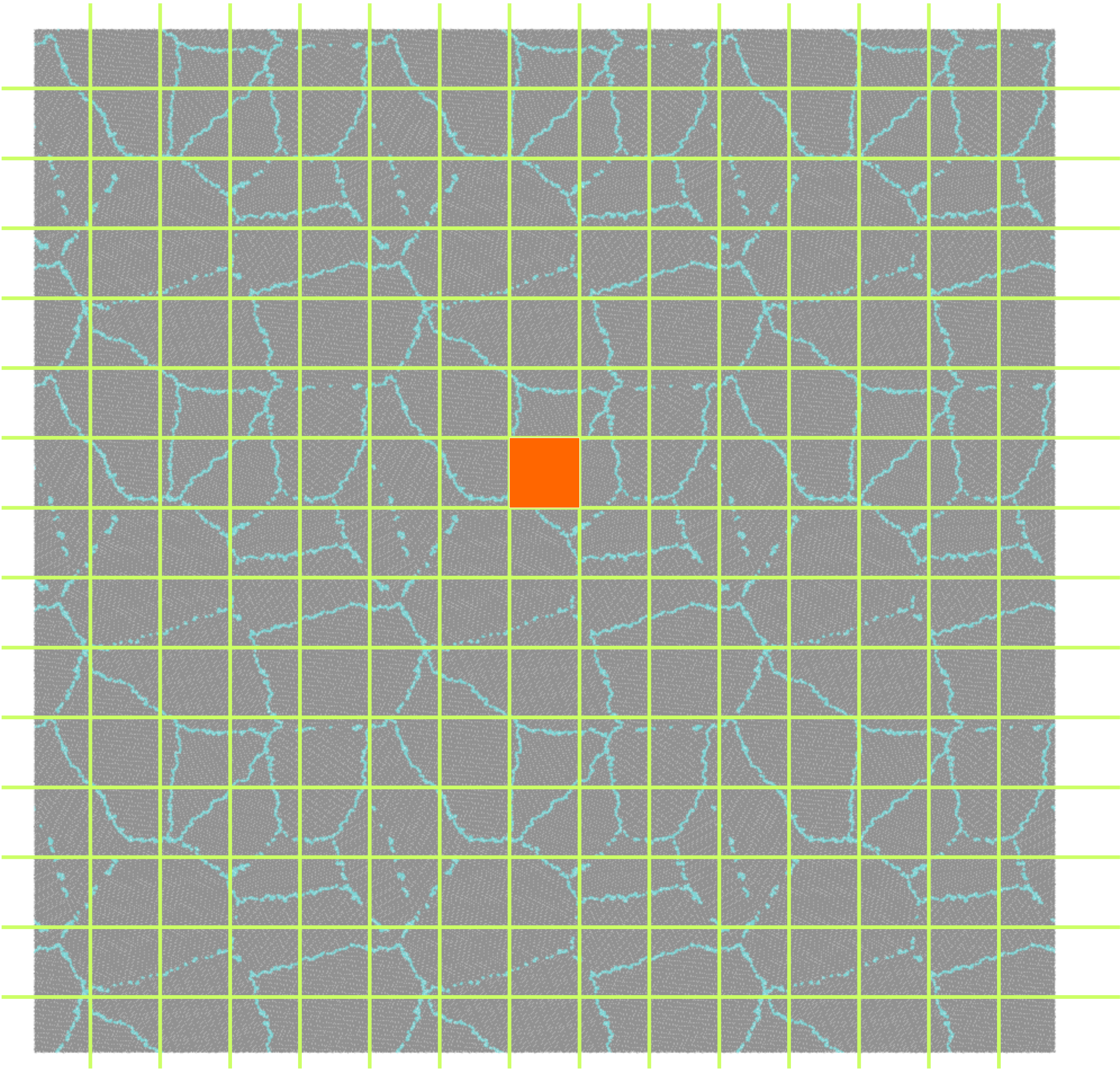

- Cells(i, j, #)

- Busqueda de vecinos

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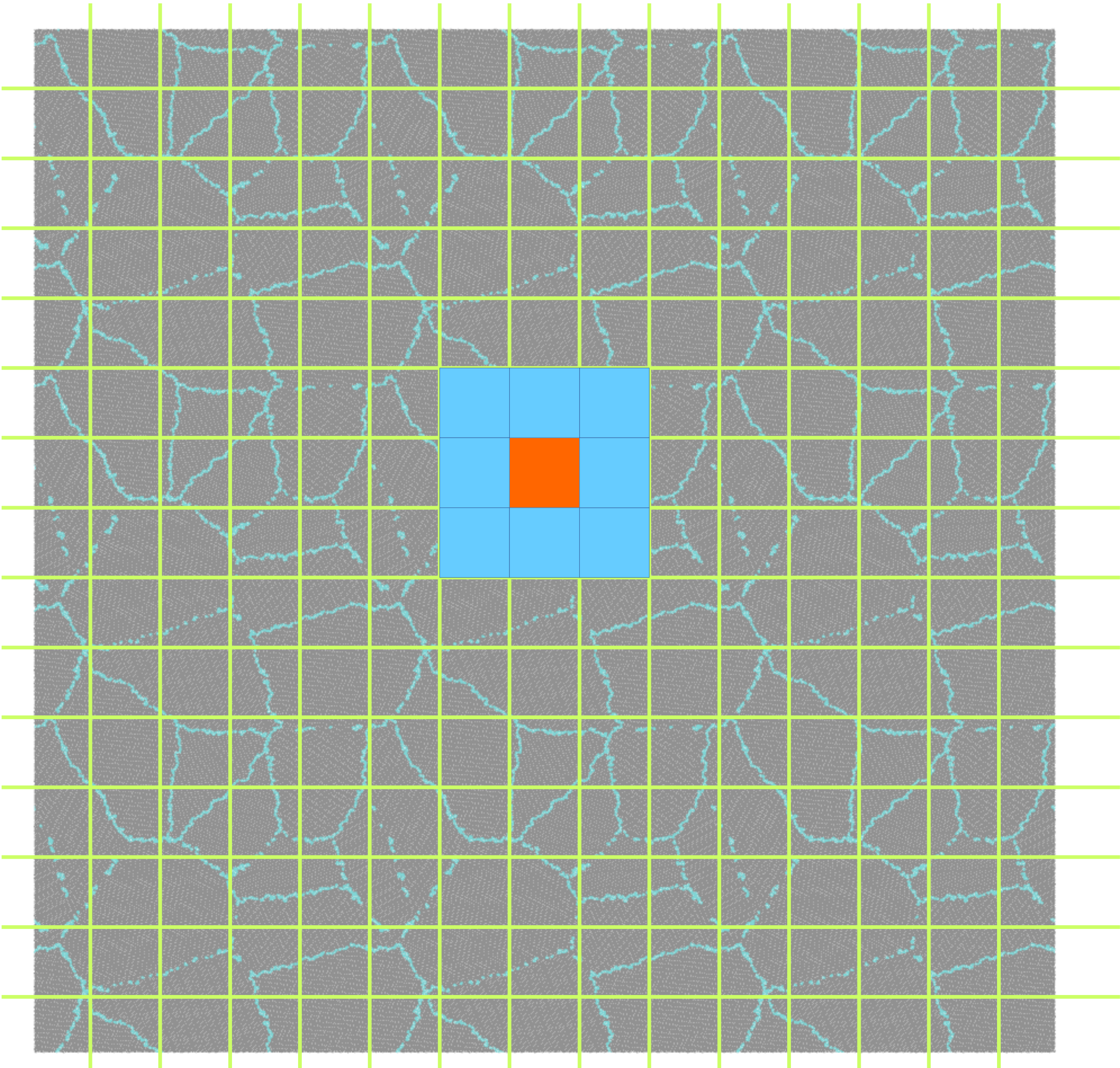

- Cells(i, j, #)

- Búsqueda de vecinos

- Cada búsqueda es independiente

Operador evolución (receta)

$$|\Psi(t)\rangle = \mathrm{e}^{-i\mathcal{H}t/\hbar}|\Psi(0)\rangle$$

$$\mathrm{e}^{-i\mathcal{H}t} = J_0(t) + 2\sum_{m=1}^{\infty}(-i)^m J_m(t) T_m(\mathcal{H})$$

(1) Estado inicial

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(2) Coeficientes → funciones de Bessel

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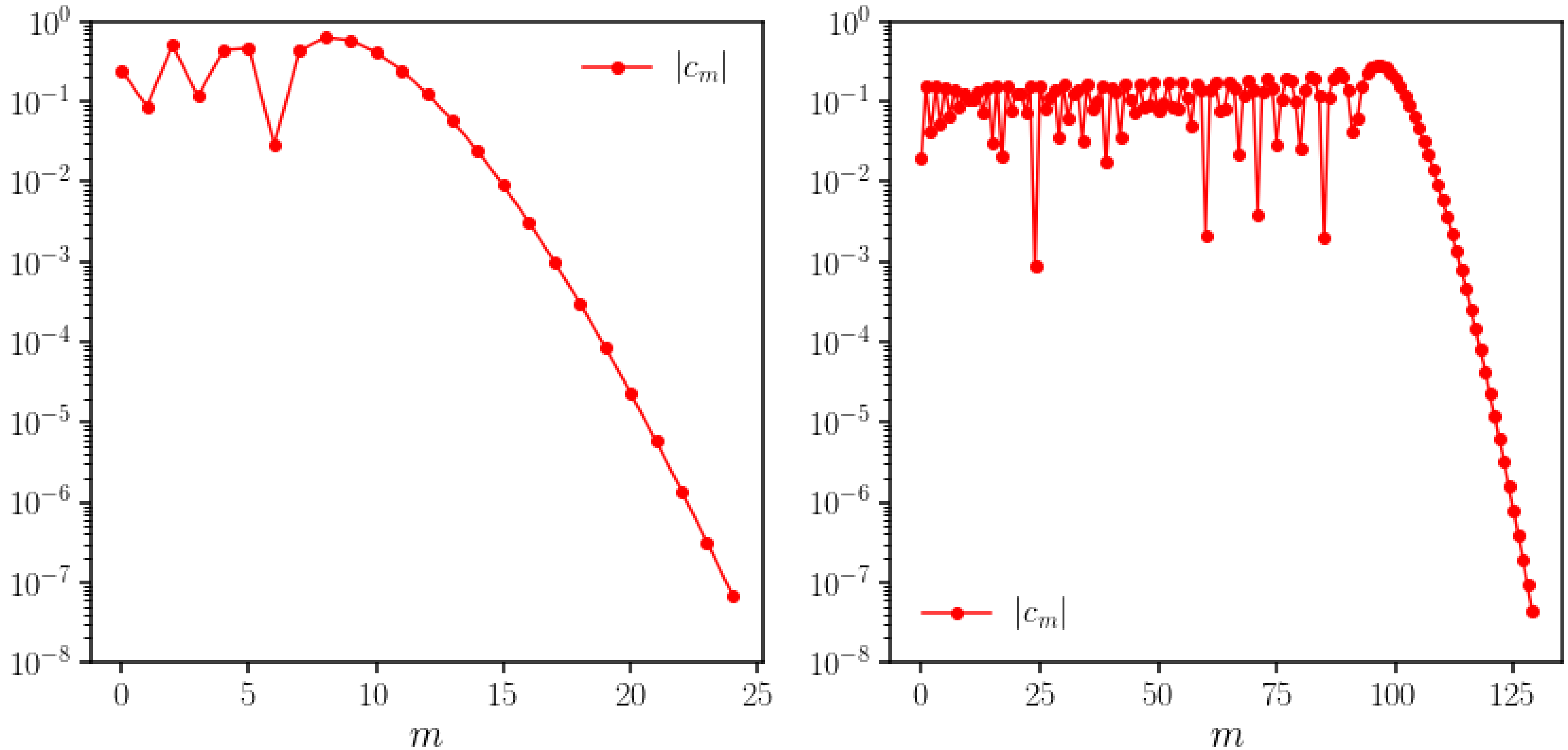

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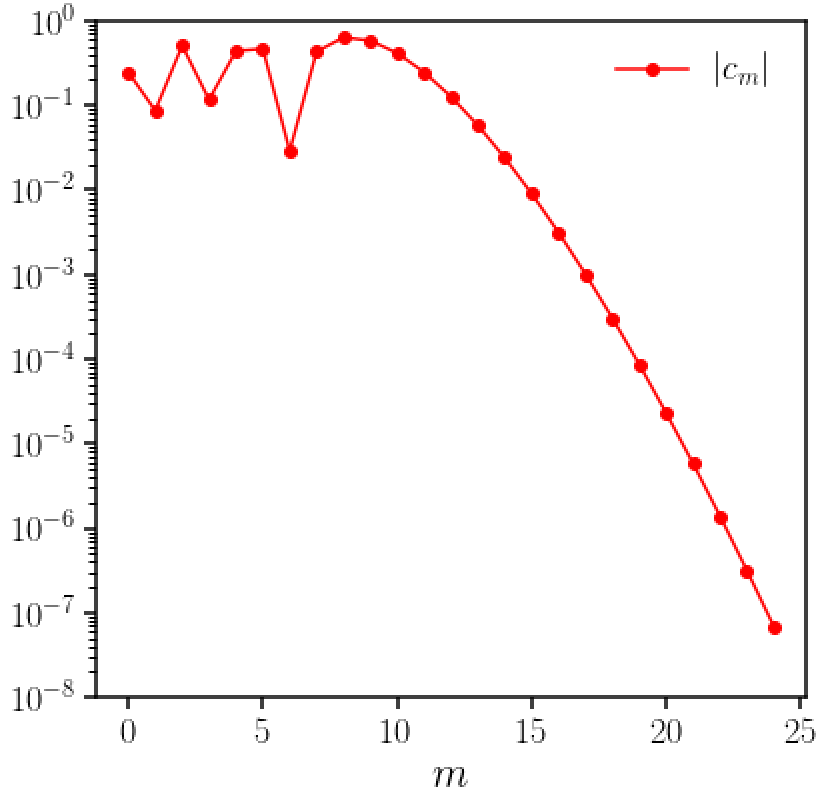
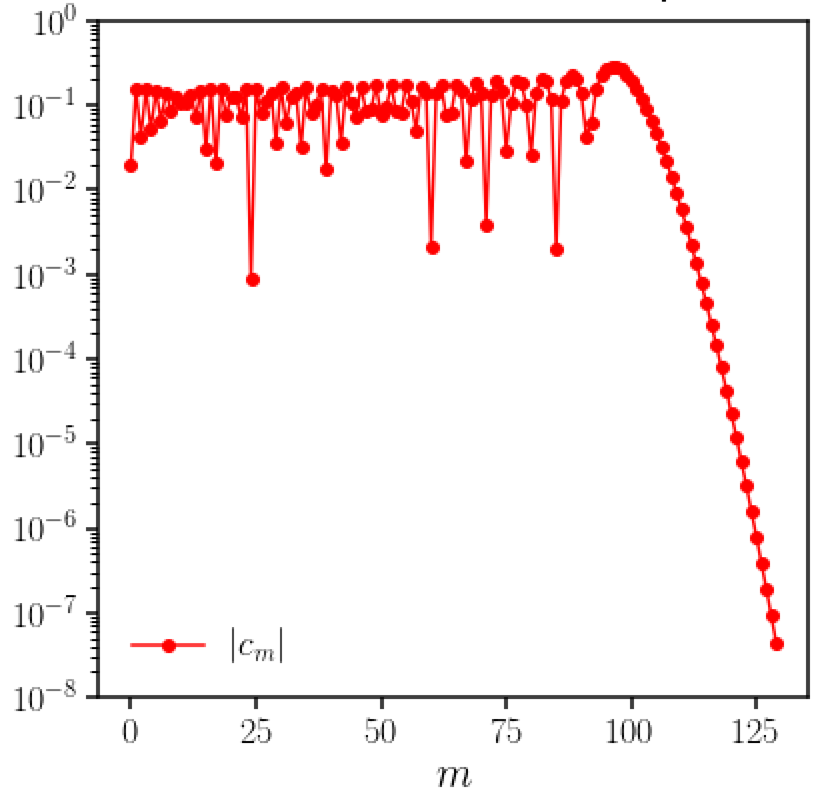
OBS:
Pasos de tiempo largos





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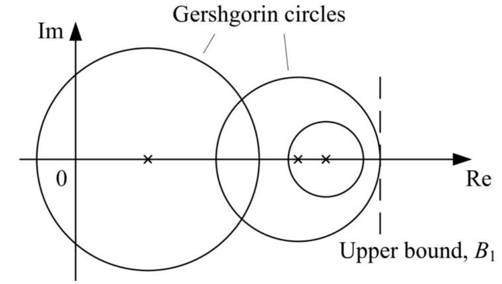
OBS:
Teorema de Gershgoring



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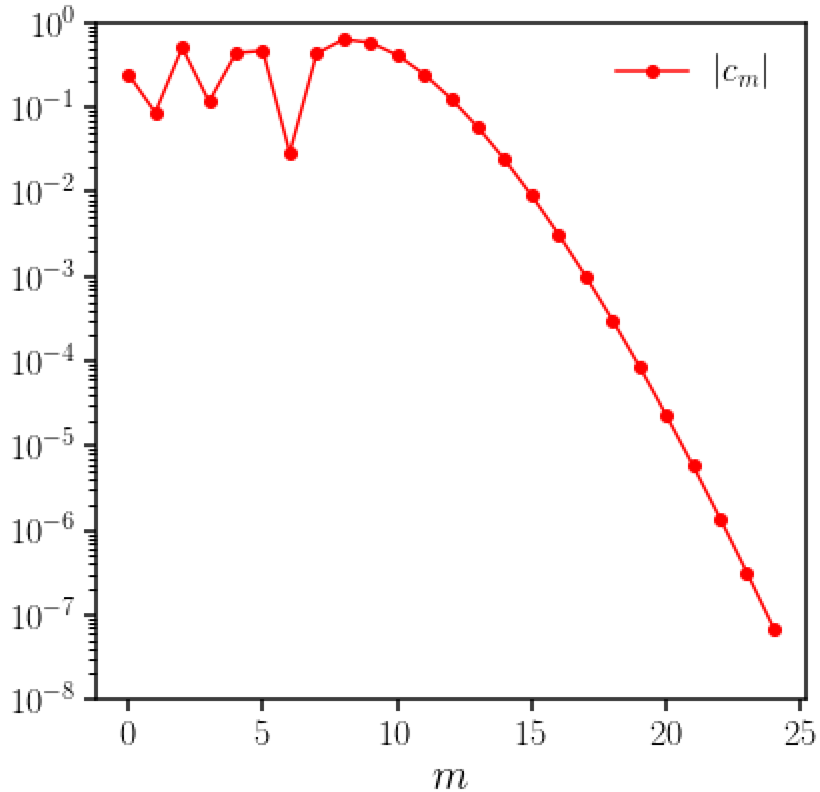

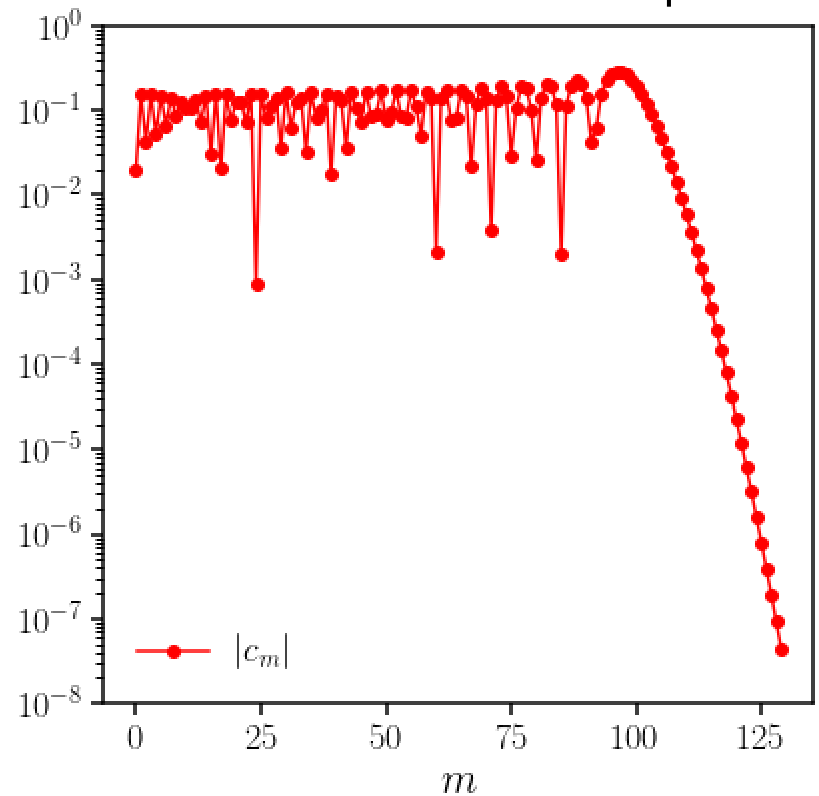

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(3) Recursion → Chebyshev polynomials

Operador evolución (receta)

$$|\Psi(t)\rangle = \mathrm{e}^{-i\mathcal{H}t/\hbar}|\Psi(0)\rangle$$

$$\mathrm{e}^{-i\mathcal{H}t} = J_0(t) + 2\sum_{m=1}^{\infty}(-i)^m J_m(t) T_m(\mathcal{H})$$

(3) Recursion → Chebyshev polynomials

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$$T_1(H) = H$$

$$T_2(H) = 2H^2 - H$$

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$$\Downarrow$$

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↓

$$|r_n\rangle = 2H|r_{n-1}\rangle - |r_{n-2}\rangle$$


PAUSE
RELAX
THINK

Funciones de Green (y DOS)

Funciones de Green (y DOS)

$$\mathrm{DOS}(E) = -\frac{1}{\pi}\mathrm{Im}\,\mathrm{Tr}\left\{G(E)\right\}$$

$$G(E) = \frac{1}{E + i\eta - \hat{H}} \xrightarrow[\eta \to 0]{} \delta(E - \hat{H})$$

Expansión en polinomios (Delta de Dirac)

$$f(x) \approx \frac{1}{\pi\sqrt{1-x^2}}\left(\mu_0 + 2\sum_{n=1}^{N-1} \mu_n T_n(x)\right), \quad \mu_n = \int_{-1}^{1} f(x) T_n(x) dx\,.$$

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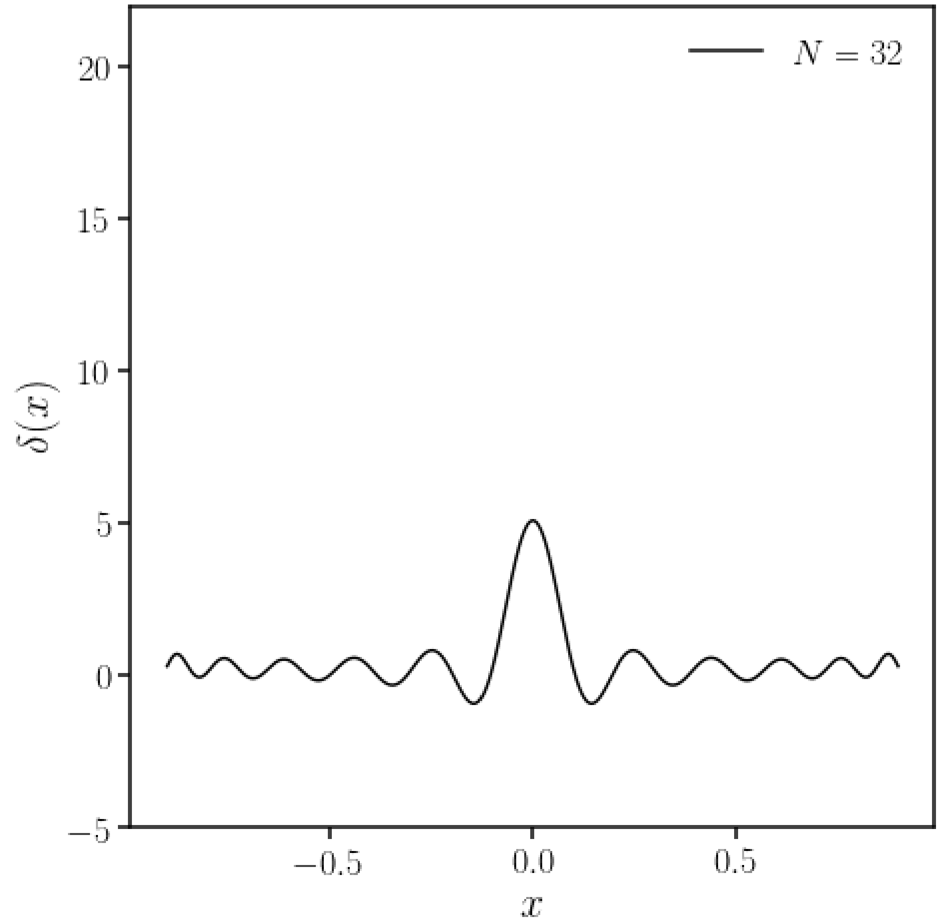

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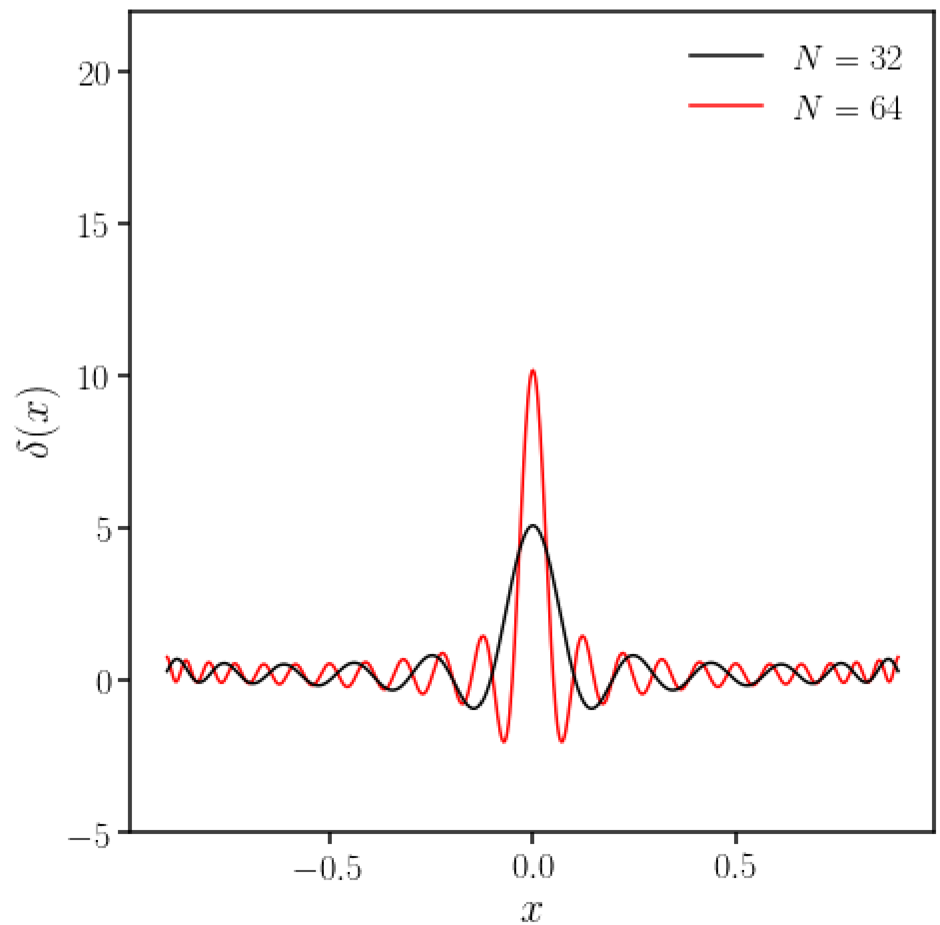

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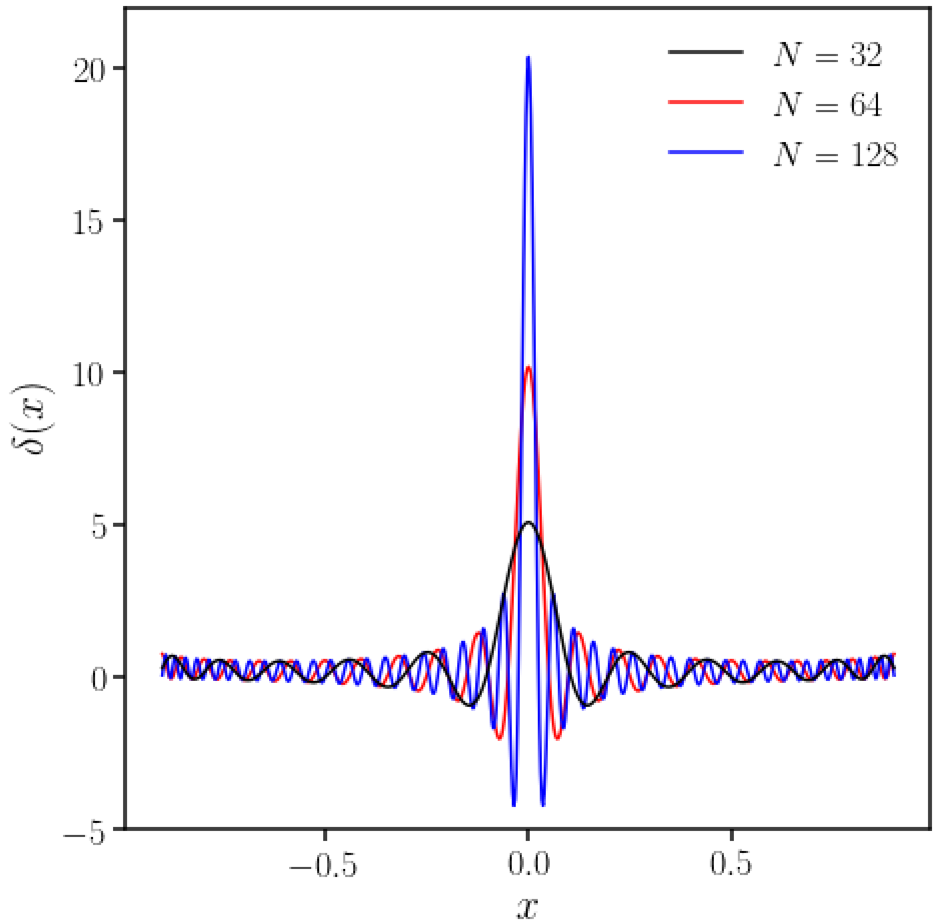

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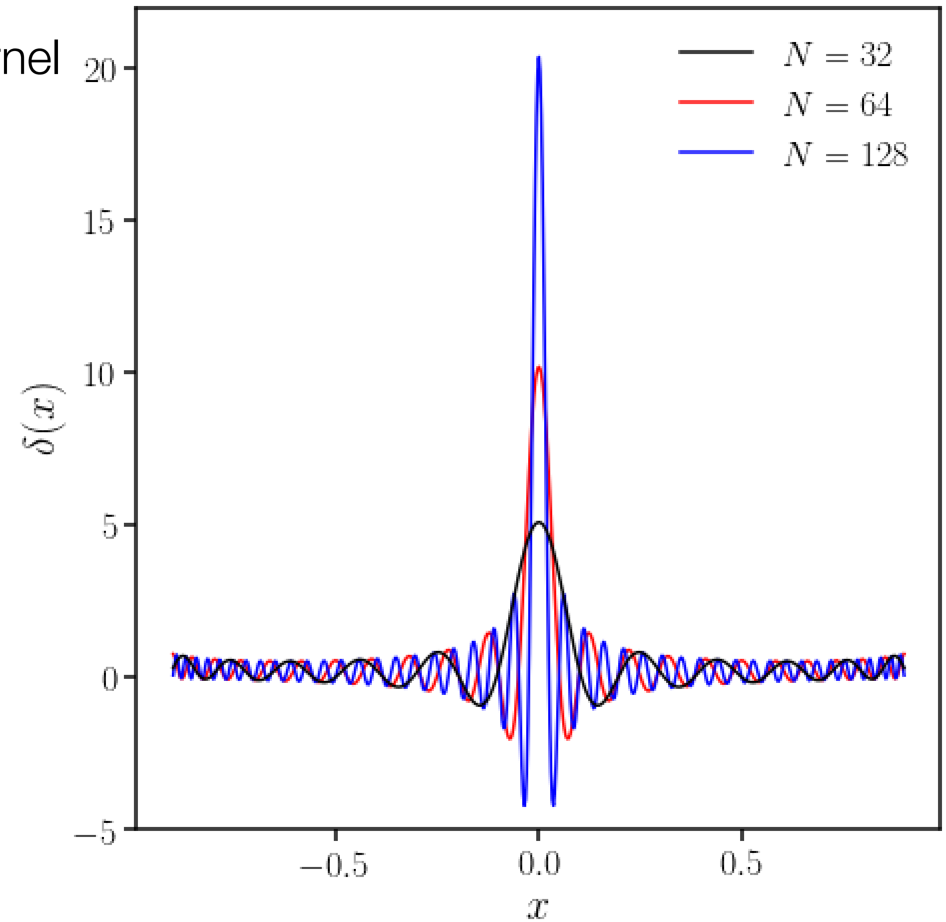
$$\times g_n$$

OBS: Serie finita → Kernel



Expansión en polinomios

$$f(x_k) = \frac{1}{\pi\sqrt{1-x_k^2}}\left(g_0\mu_0 + 2\sum_{n=1}^{N-1} g_n\mu_n T_n(x_k)\right). \qquad \mu_n = \int_{-1}^{1} f(x)\,T_n(x)\,dx\,.$$

OBS: Serie finita → Kernel

Name	g_n	Parameters	positive?	Remarks
Jackson	$\frac{1}{N+1}\left[(N-n+1)\cos\frac{\pi n}{N+1} + \sin\frac{\pi n}{N+1}\cot\frac{\pi}{N+1}\right]$	none	yes	best for most applications
Lorentz	$\sinh[\lambda(1-n/N)]/\sinh(\lambda)$	$\lambda \in \mathbb{R}$	yes	best for Green functions
Fejér	$1-n/N$	none	yes	mainly of academic interest
Lanczos	$\left(\frac{\sin(\pi n/N)}{\pi n/N}\right)^M$	$M \in \mathbb{N}$	no	$M=3$ closely matches the Jackson kernel, but not strictly positive (Lanczos, 1966)
Wang and Zunger	$\exp\left[-\left(\alpha\frac{n}{N}\right)^\beta\right]$	$\alpha,\beta \in \mathbb{R}$	no	found empirically, not optimal (Wang, 1994; Wang and Zunger, 1994)
Dirichlet	1	none	no	least favorable choice

Alexander Weiße et al.. The kernel polynomial method, Rev. Mod. Phys. 78, 275 (2006)

Expansión en polinomios

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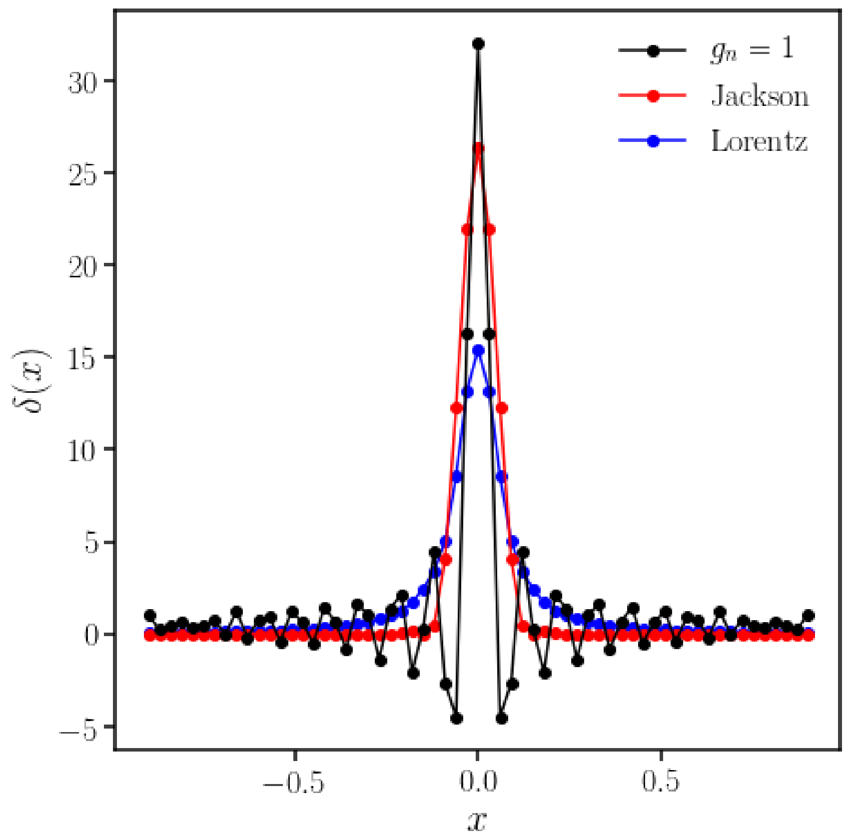

Density of States

$$\mathrm{Tr}\left\{\delta(E-H)\right\} = \frac{1}{\pi\sqrt{1-E^2}}\left[\mu_1^{\mathrm{psi}} + 2\sum_{n=2}^{\infty}\mu_n^{\mathrm{psi}}T_n(E)\right]$$

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OBS: Stochastic evaluation

$$|\psi_{\mathrm{RP}}\rangle = \frac{1}{\sqrt{\mathrm{Nsites}}}\sum_{J=1}^{\mathrm{Nsites}} \mathrm{e}^{i2\pi\theta_J}|J\rangle$$

$$\mu_n^{\mathrm{psi}} = \langle\psi_{\mathrm{RP}}|T_n(\mathcal{H})|\psi_{\mathrm{RP}}\rangle \times g_n$$

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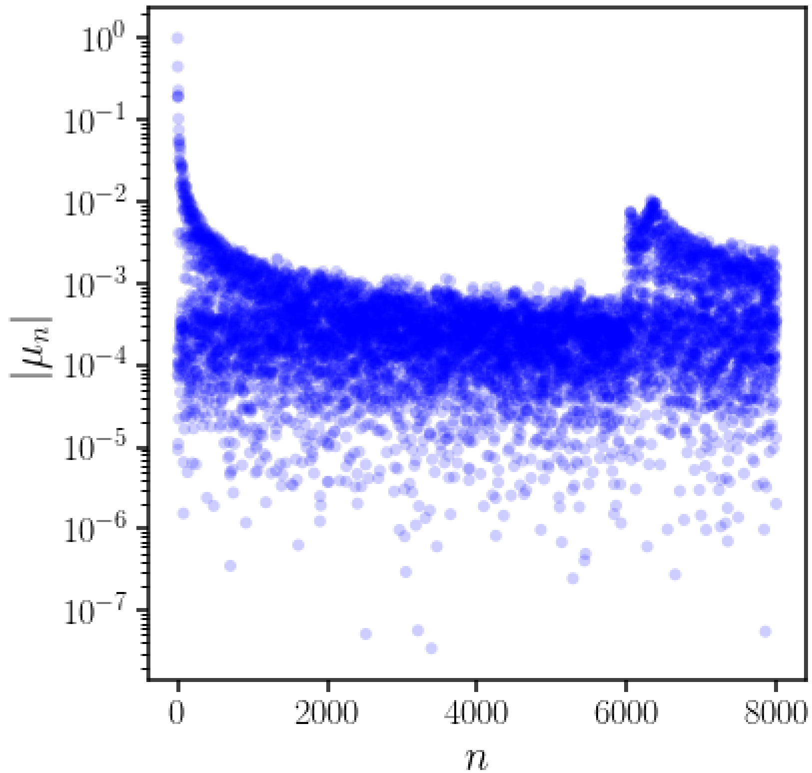
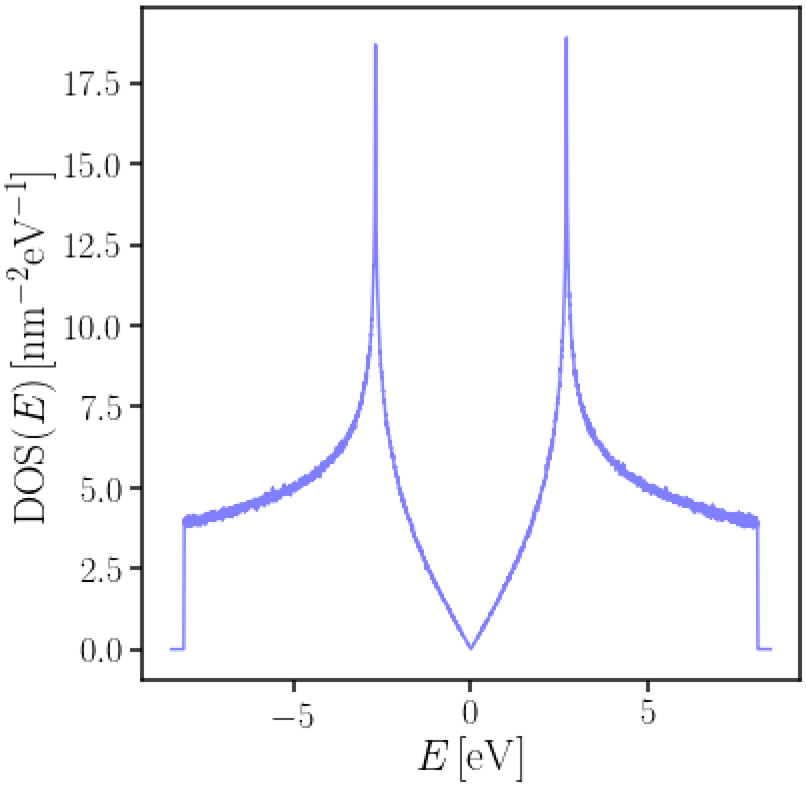




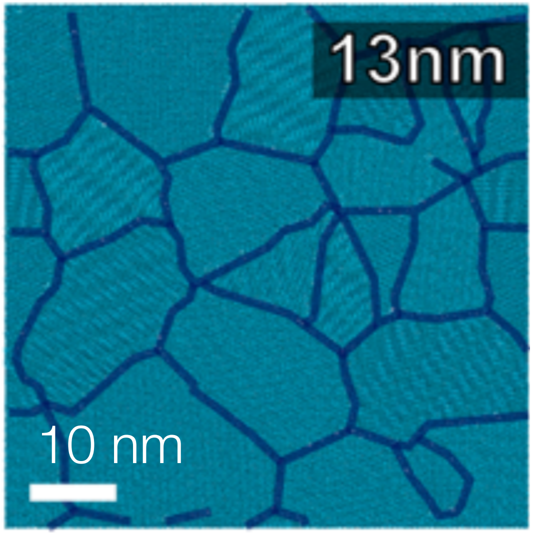
Ejemplo notebook - KPM

Resumen metodología - KPM

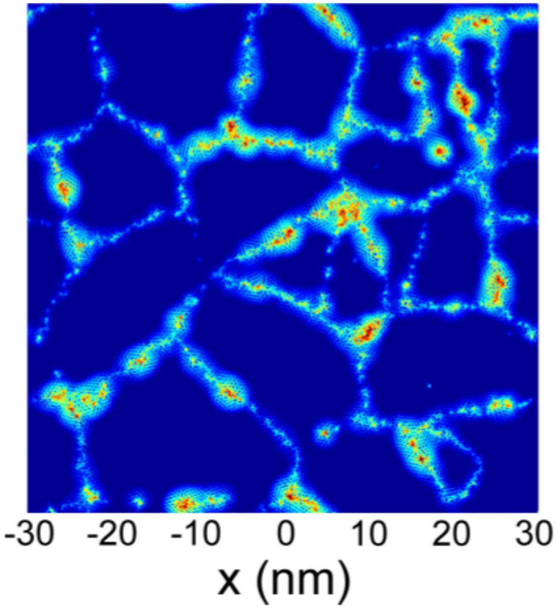
1 Red

2 Hamiltoniano

3 Transporte electrónico



$$\mathrm{LDOS}(E = 0)$$



Respuesta lineal – Fórmula de Kubo

$$\sigma \propto \int dt \langle J(t), J(0) \rangle$$

$$\sigma(E) = \frac{e^2}{2} \left[\mathrm{DOS}(E) \right] \lim_{t \to \infty} \frac{\partial}{\partial t} \left\langle \Delta X^2(t) \right\rangle_E$$

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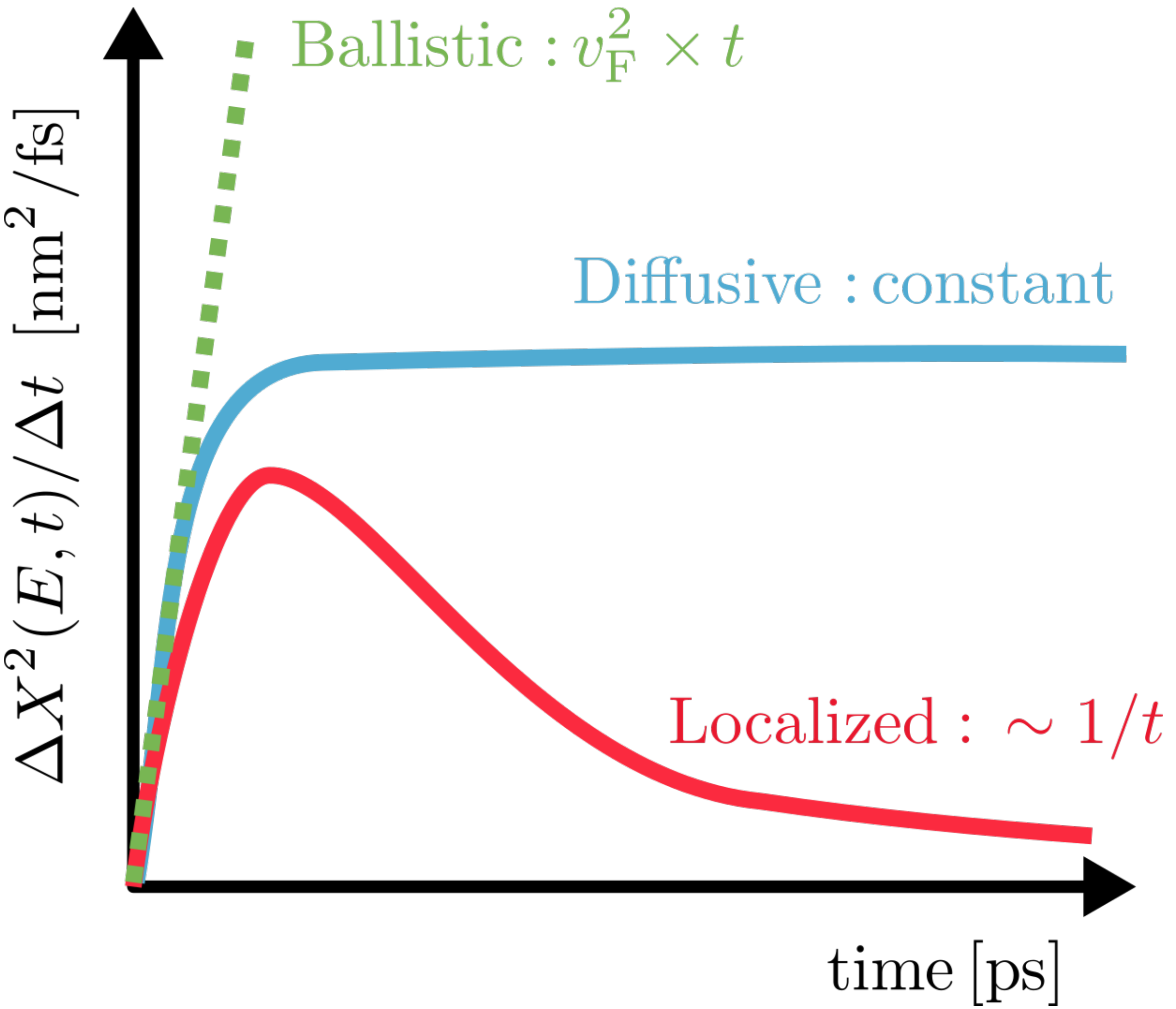

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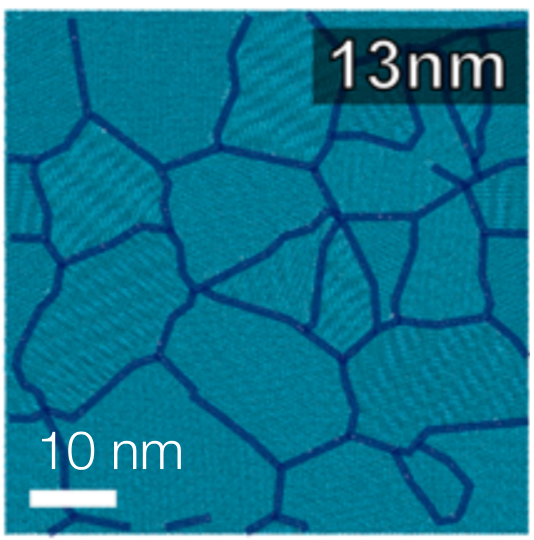

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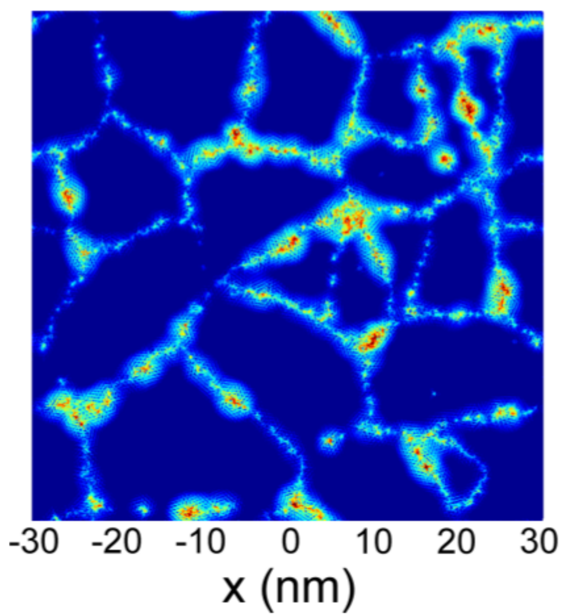

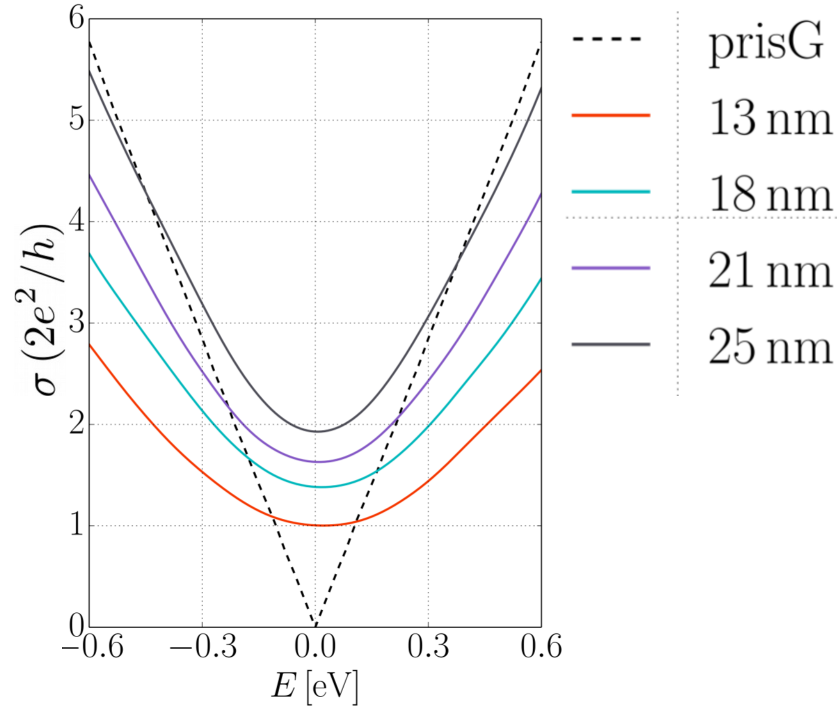

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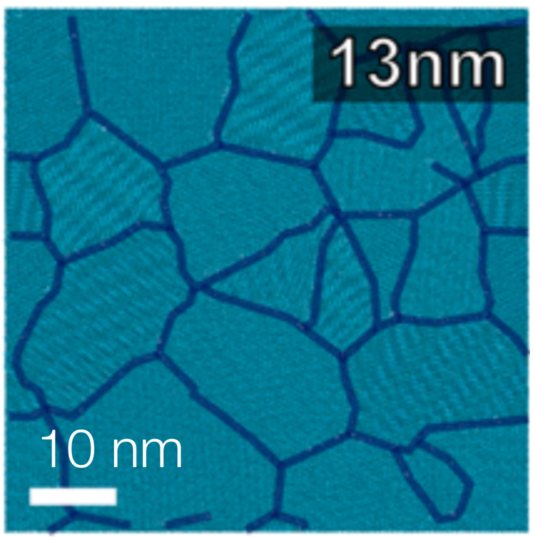
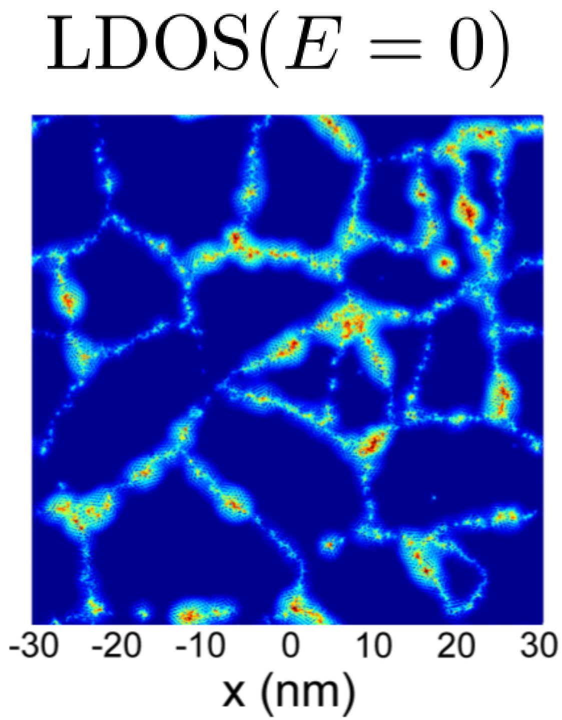
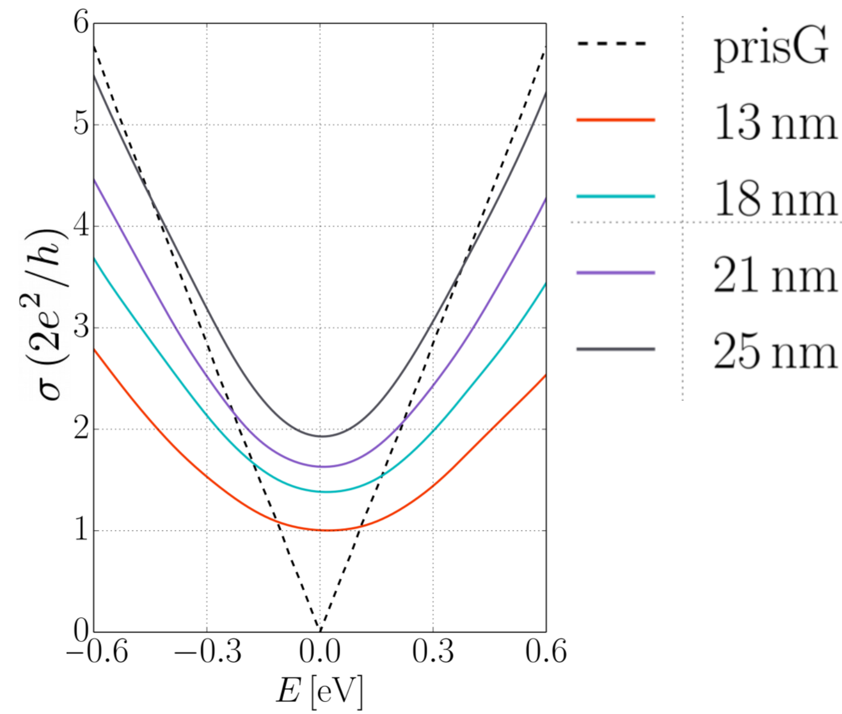
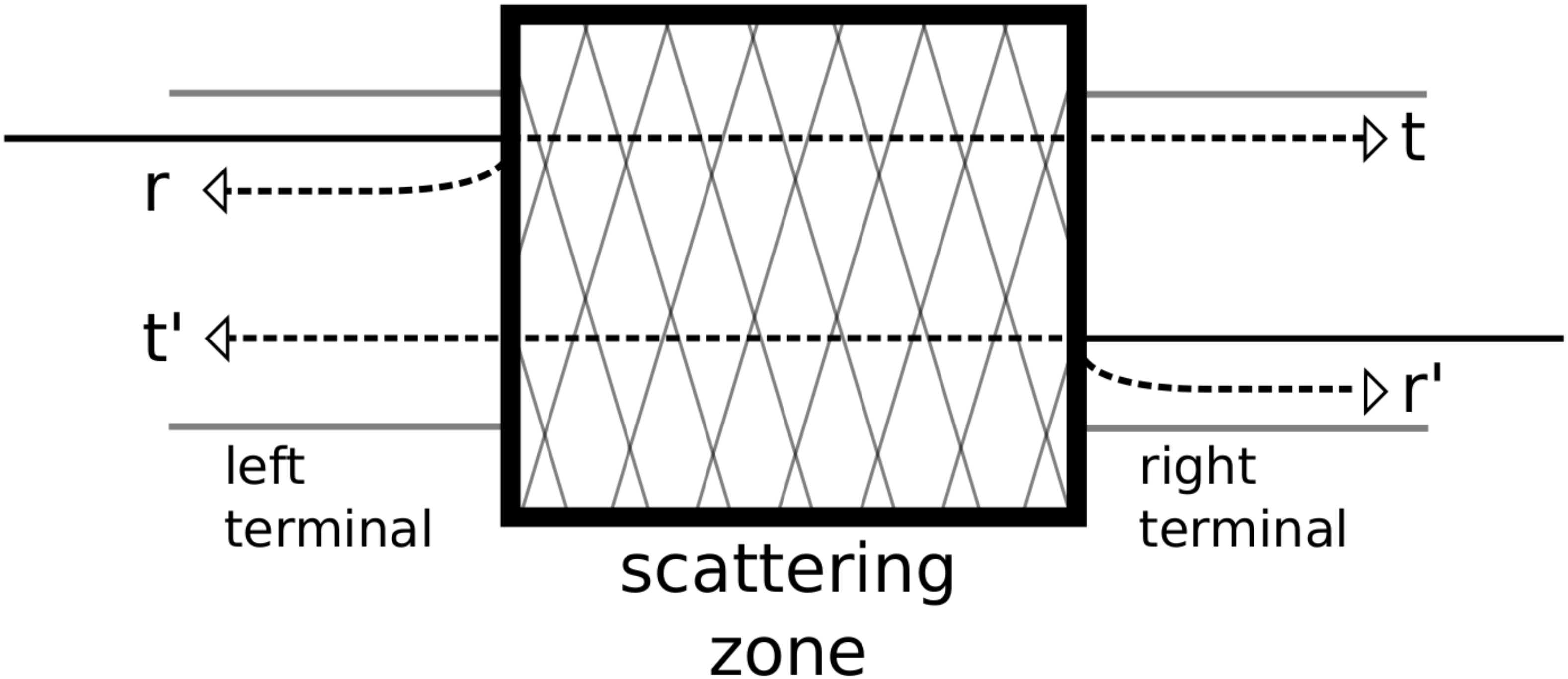






OBS: Implementación numérica de O(N) (Kernel polynomial method) kwant

kwant



$$\begin{pmatrix} c^{\text{oL}} \\ c^{\text{oR}} \end{pmatrix} = S \begin{pmatrix} c^{\text{iL}} \\ c^{\text{iR}} \end{pmatrix}. \qquad S = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix}$$

El *workflow* típico en Kwant es:

1. Crear un sistema de amarre fuerte “*empty*”.
2. Asignar los elementos de matriz y hoppings.
3. Unir los contactos (sistema de amarre fuert con simetría traslacional).
4. Enviar el sistema finalizado al *solver.*

Fase de Peierls

$$t_{ij} = -t \exp\left(i \frac{2\pi}{\Phi_0} \int_{\vec{r}_i}^{\vec{r}_j} \vec{A} \cdot d\vec{\ell} \right)$$

Ribbon zig-zag 100 x 100 (unidades de red)
100 Teslas