XXXI Simposio Peruano de Física

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Universidad Nacional Mayor de San Marcos
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Propiedades electrónicas y magnéticas de canales de grafeno grabados en fluorografeno: Transición controlable de semiconductor a metal.

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Dr Francois Peeters (Nanjing University of...)
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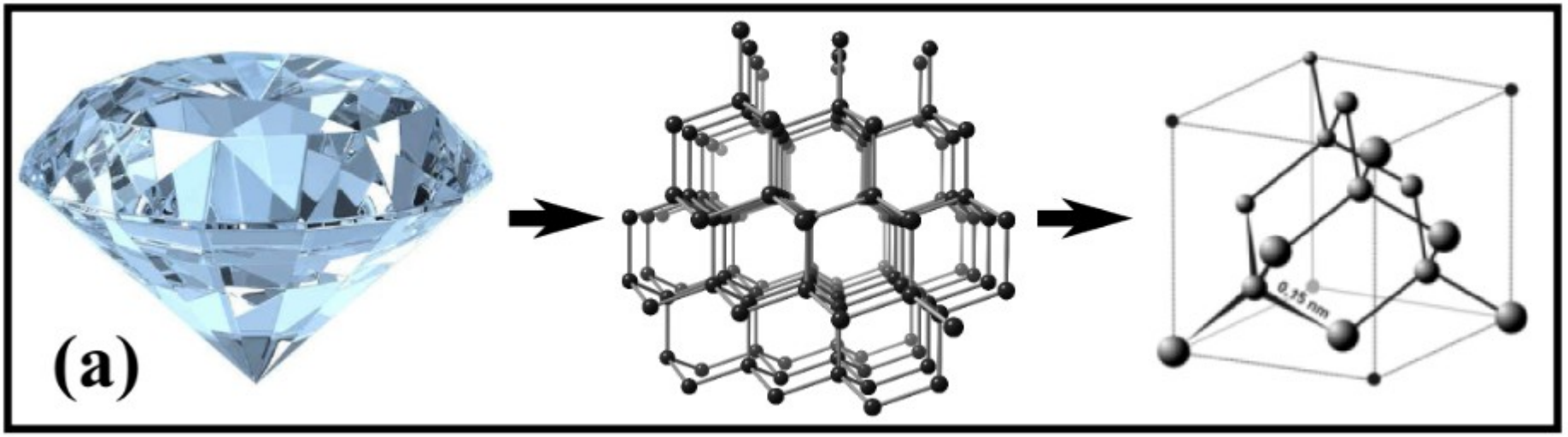
GMCAN | Grupo de Métodos Computacionales Aplicado a Nanomateriales

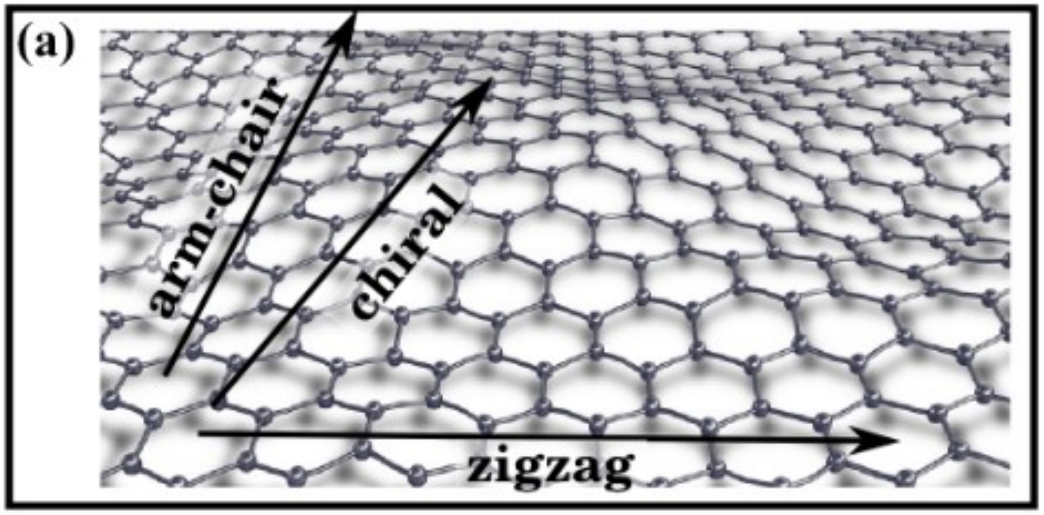
Organización

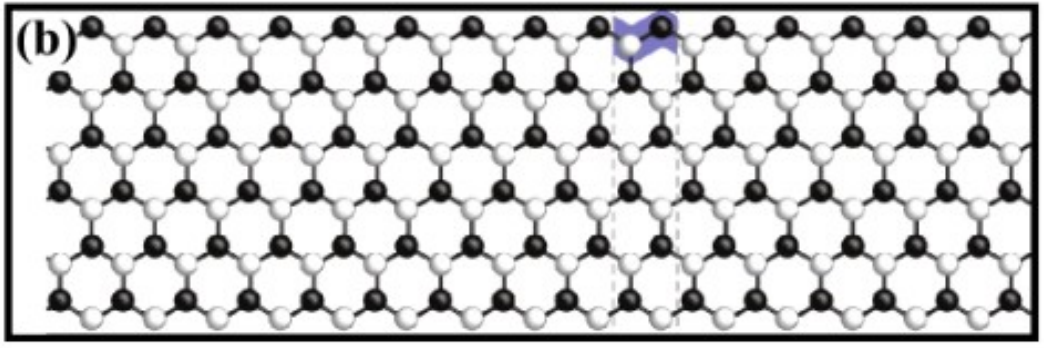
1) Compuestos de Carbono.
2) Grafeno – Nano cintas de grafeno.
3) Fluorografeno.
4) Canales de Grafeno – Resultados de primeros principios.
5) Ajuste de Wannier – Verificación de parámetros.
6) Modelo de Hubbard y método Hartree-Fock.
7) Ajuste de los resultados DFT.
8) Conclusiones – Referencias.

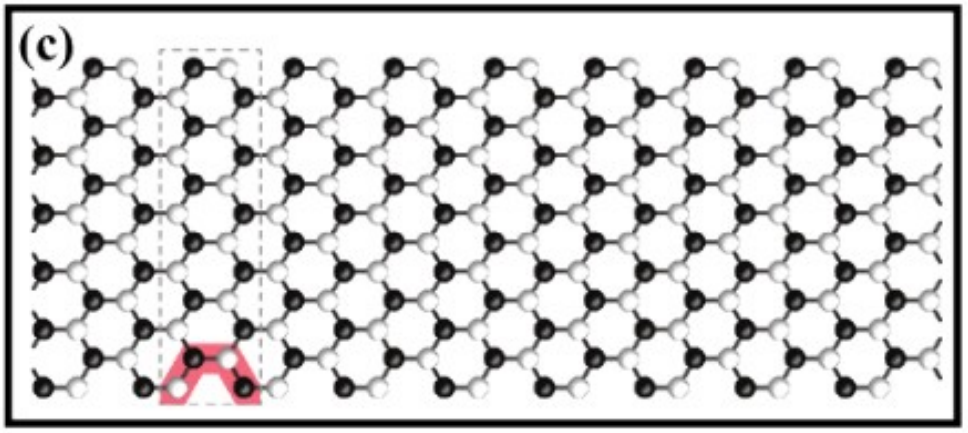
Compuestos de Carbono.

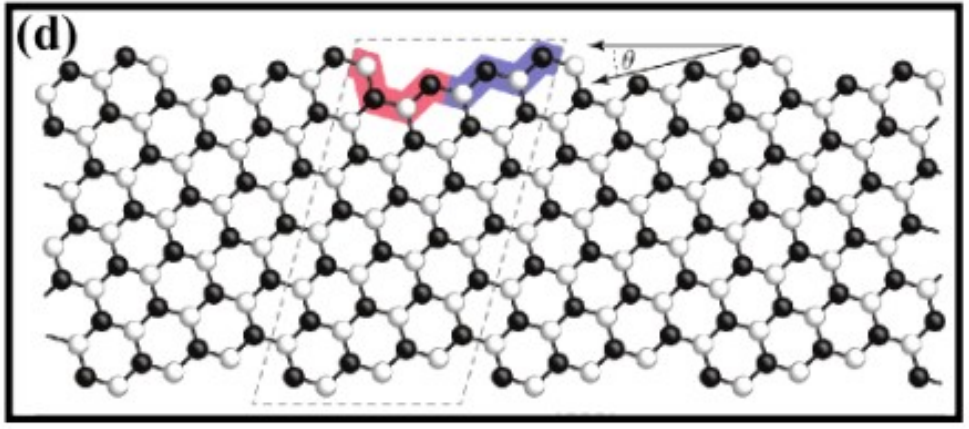


Grafeno – Nano cintas de grafeno









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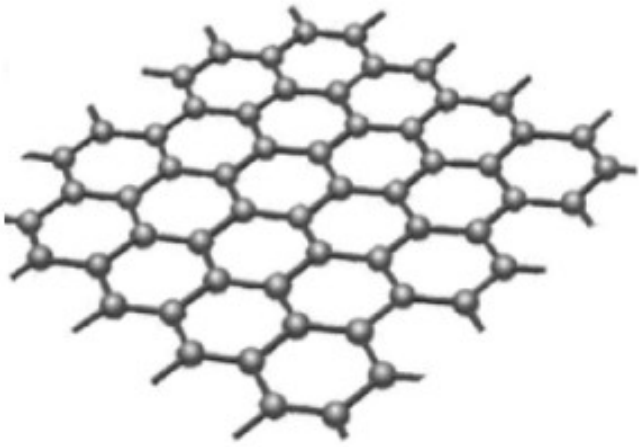
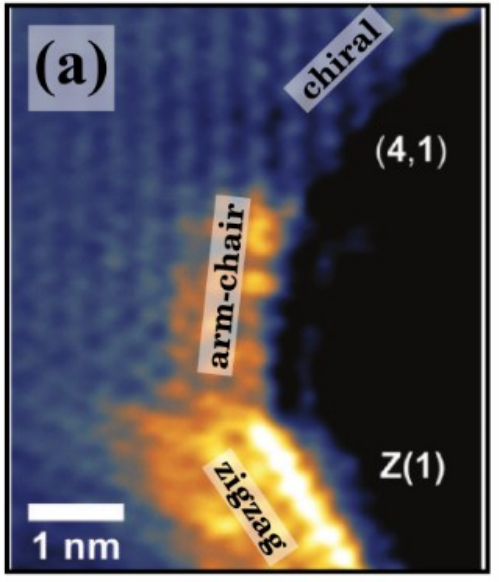
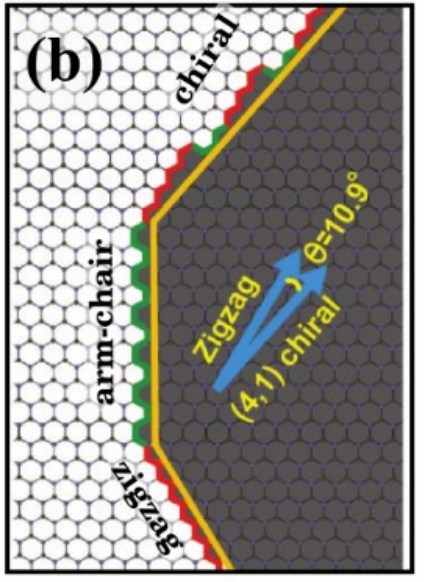
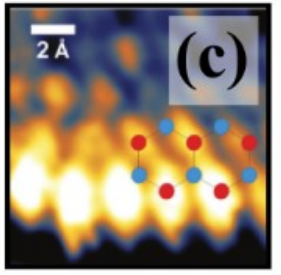
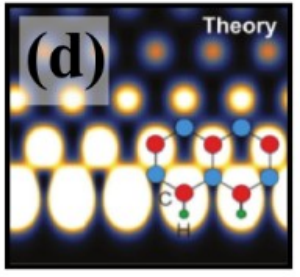
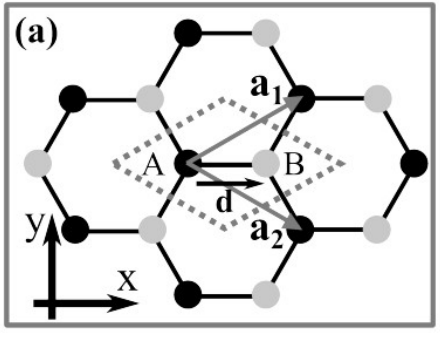


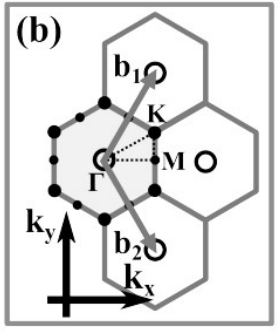


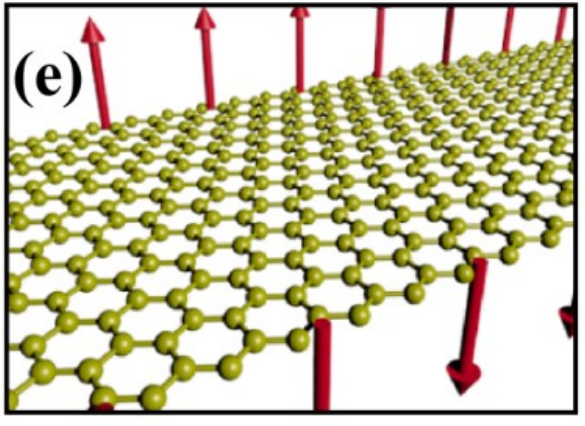


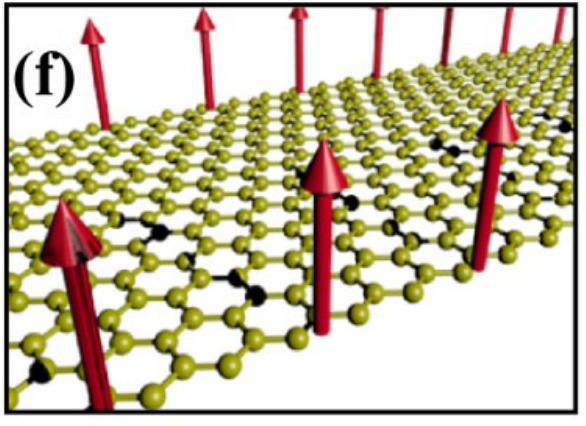




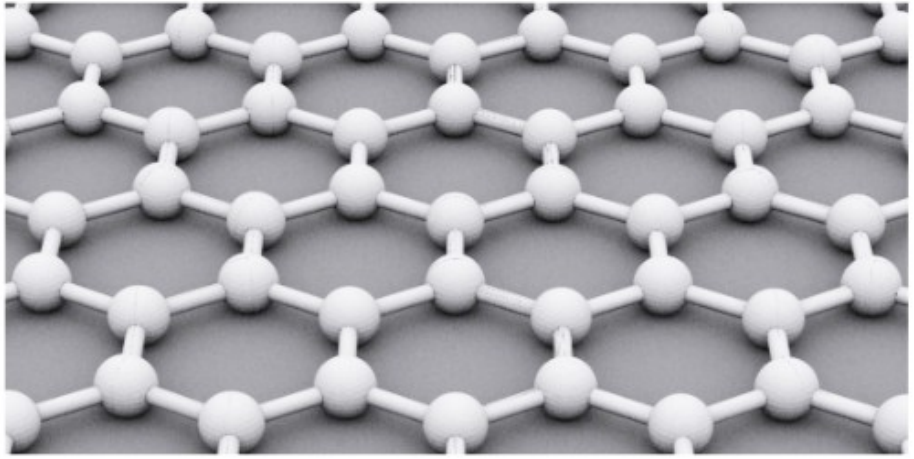


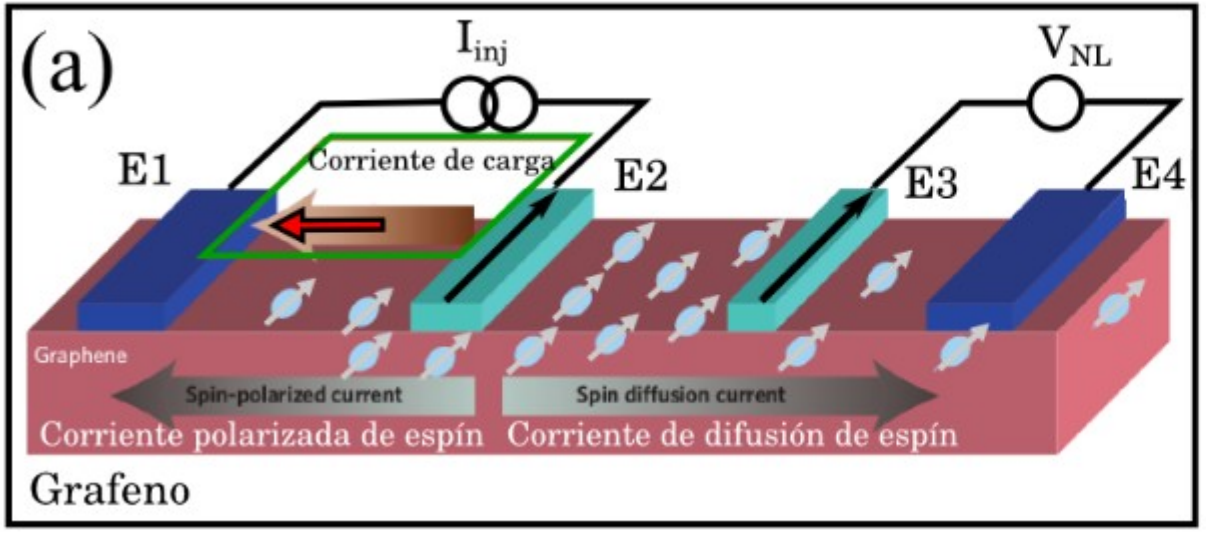


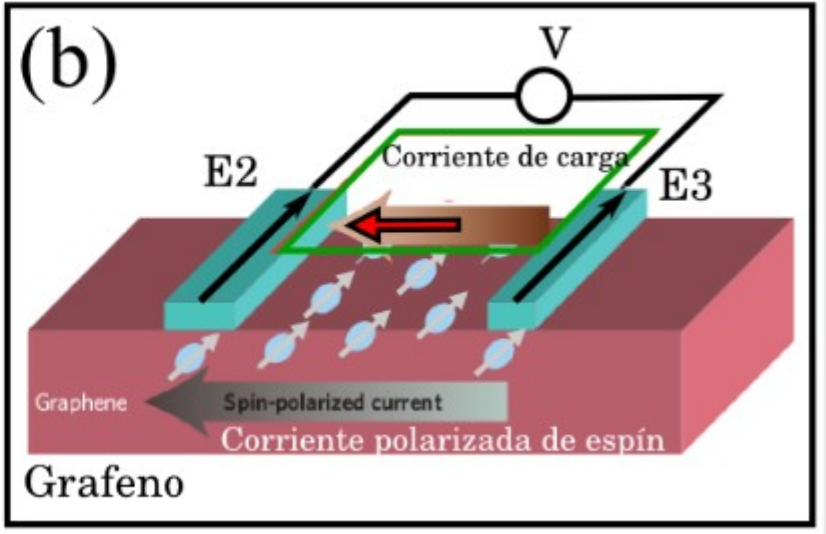




Grafeno – Nano cintas de grafeno







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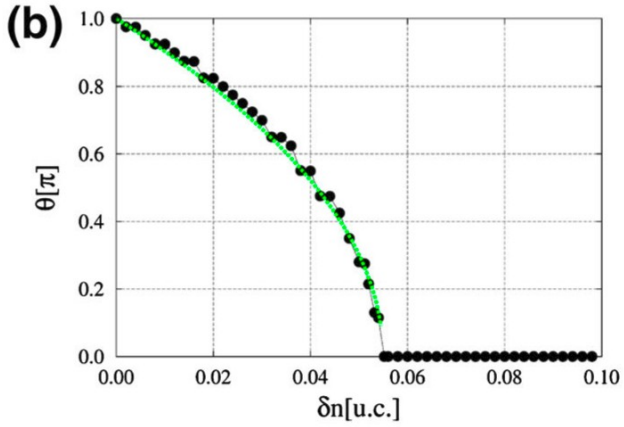
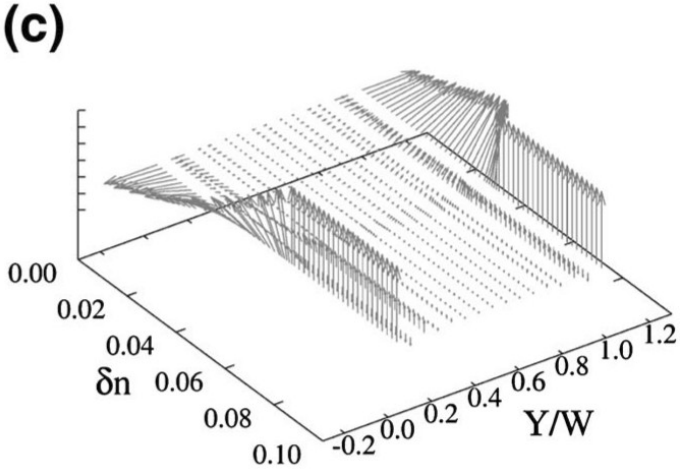
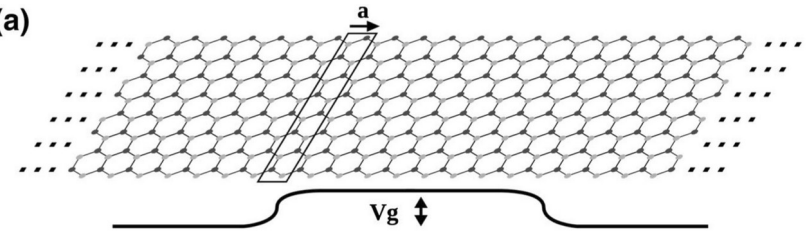




Transmission Through Gate-Induced Magnetic Islands on Graphene Nanoribbons

R. M. Guzmán Arellano · Gonz(a)

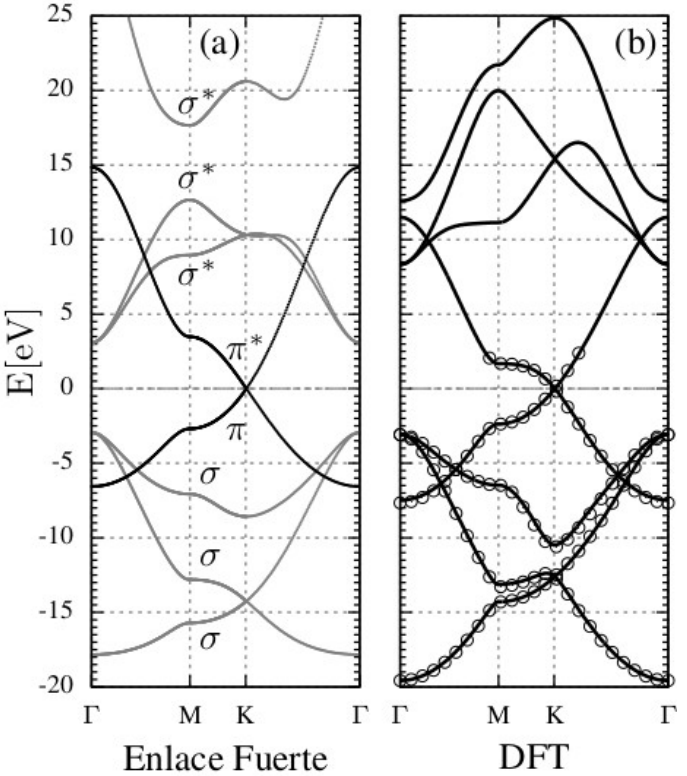


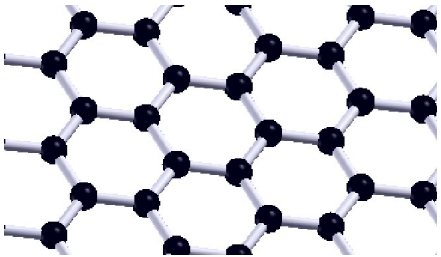
Received: 4 August 2014 / Accepted: 10 September 2014

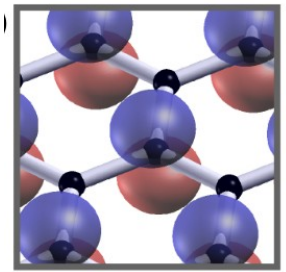
Abstract We study the spin-dependent transmission through a potential barrier in a zigzag graphene nanoribbon. In particular, we consider the effect of the magnetic order of the ribbon induced by the modulation of the local density introduced by the barrier. We model the system using an Anderson–Hubbard model that we treat in the mean field approximation. We solve this problem self-consistently and calculate the transmission coefficient using the recursive Green function method. We find that Fano-like interference dips appear on one of the spin channels as the result of the presence of spin polarized edge states in the barrier.

Keywords Graphene · Spin-dependent transport · Nanoribbons

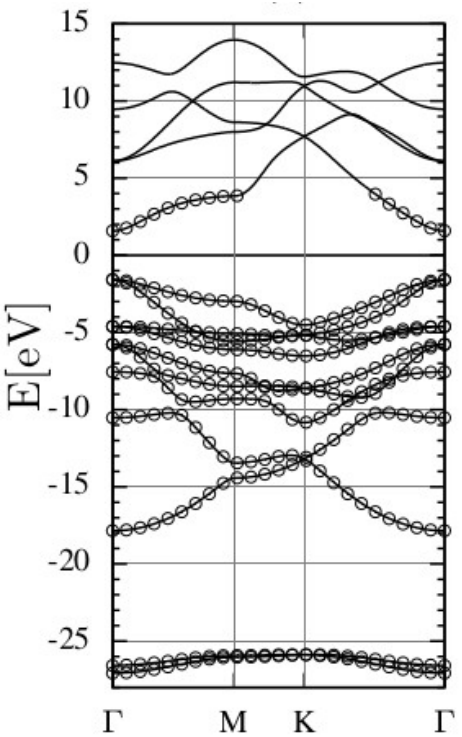
Grafeno

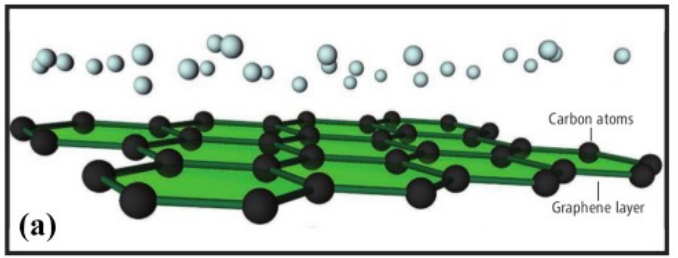


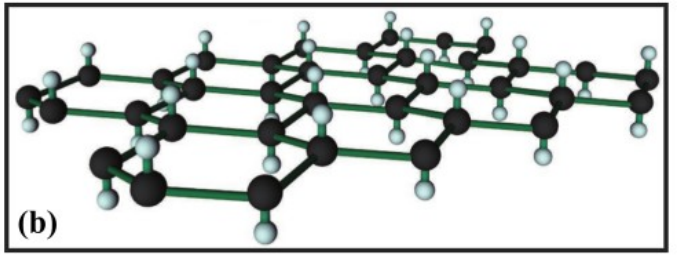


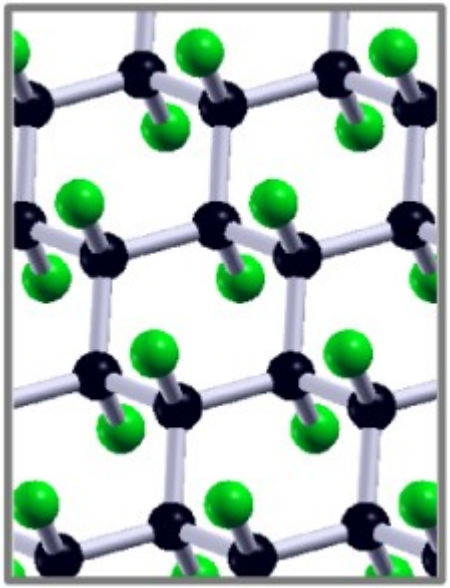


Fluorografeno

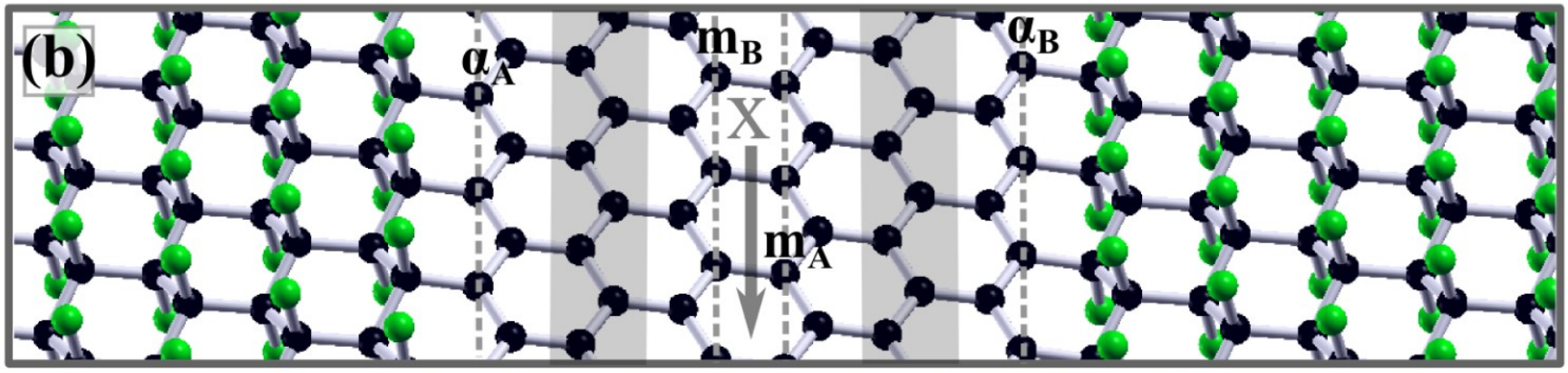


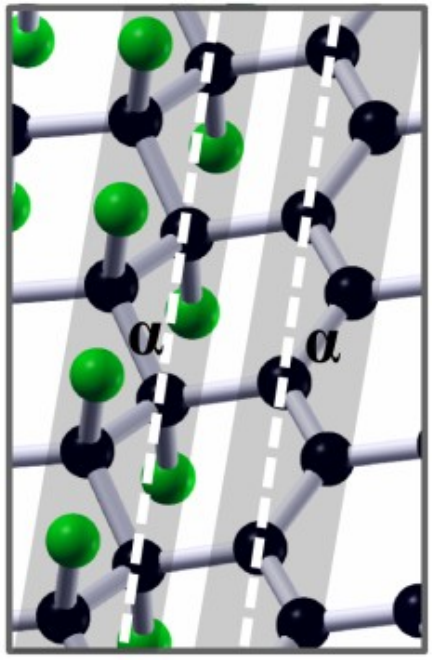


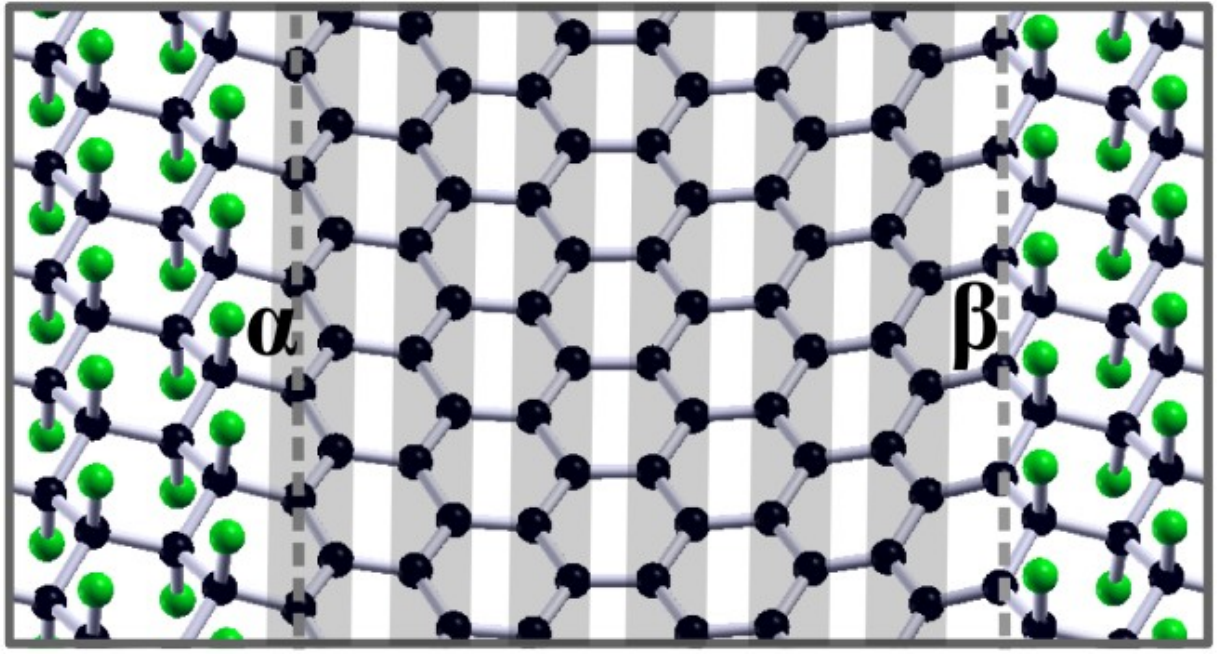


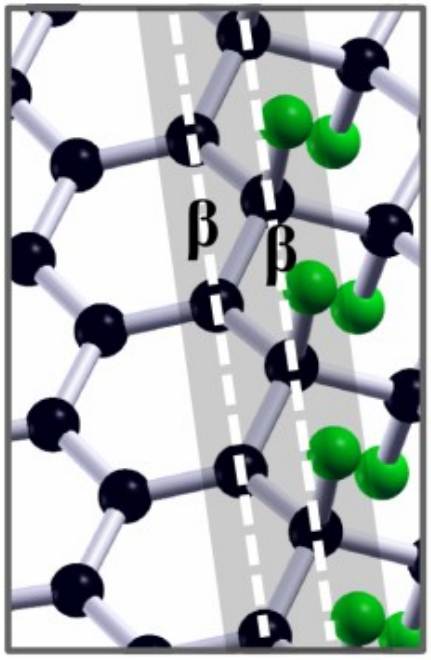


Canales de Grafeno – Resultados de primeros principios









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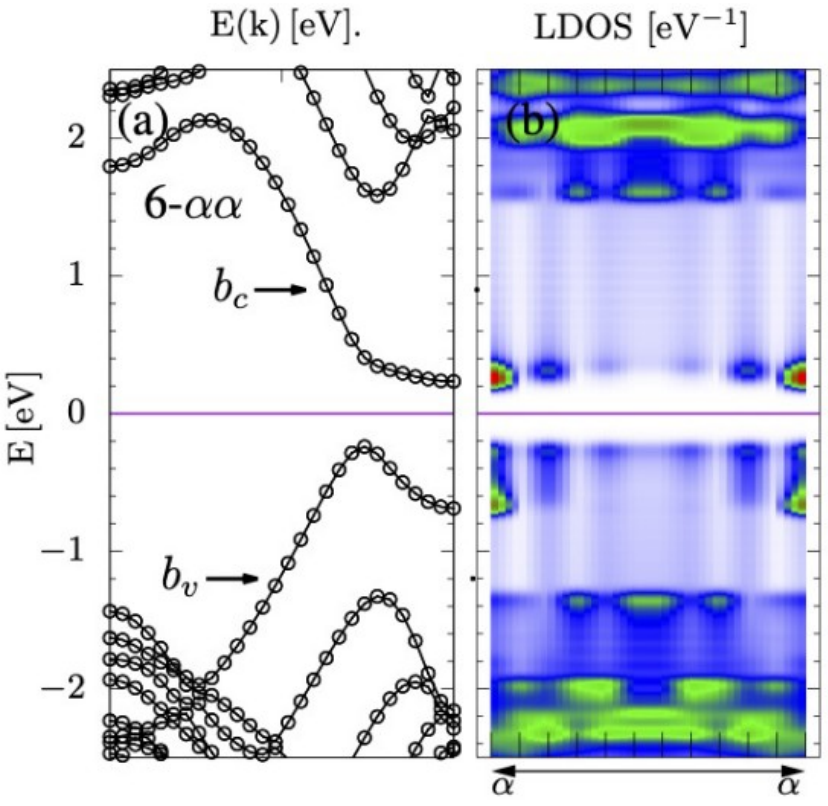
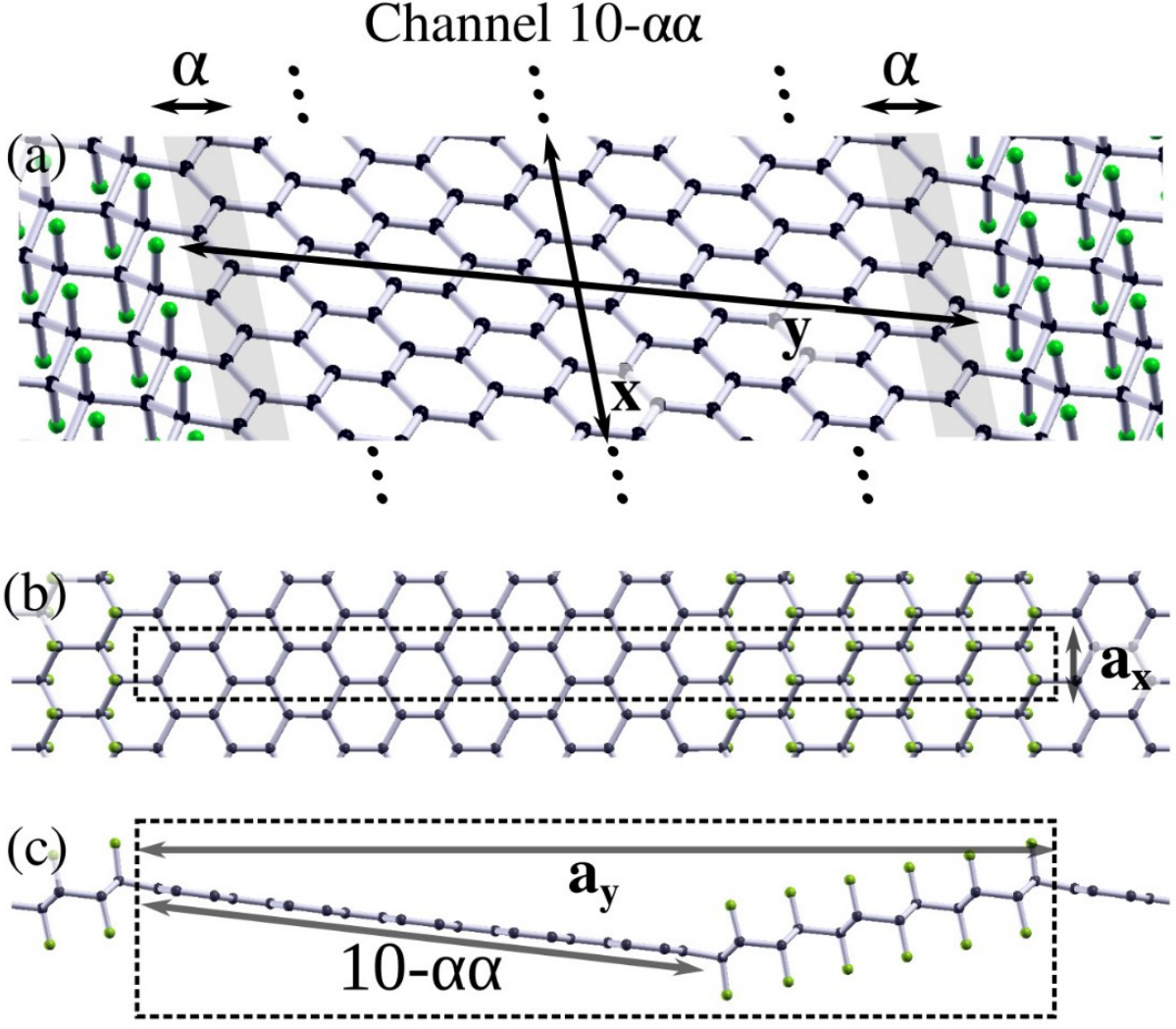
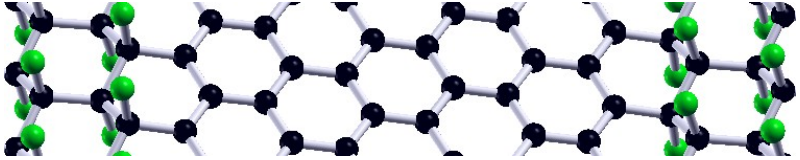
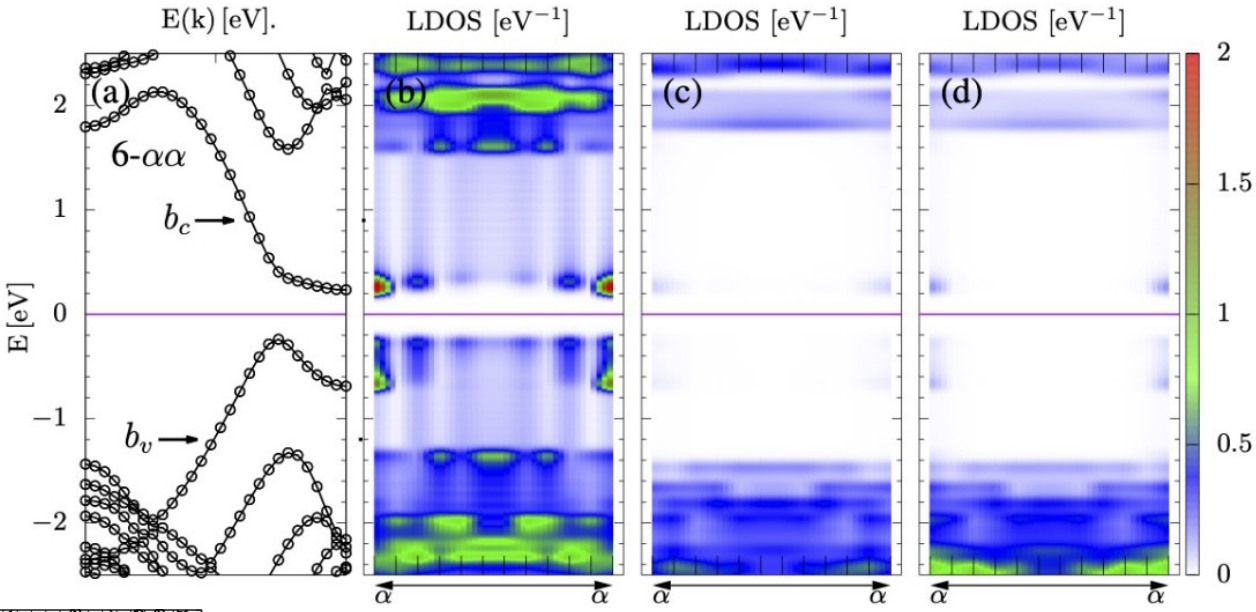


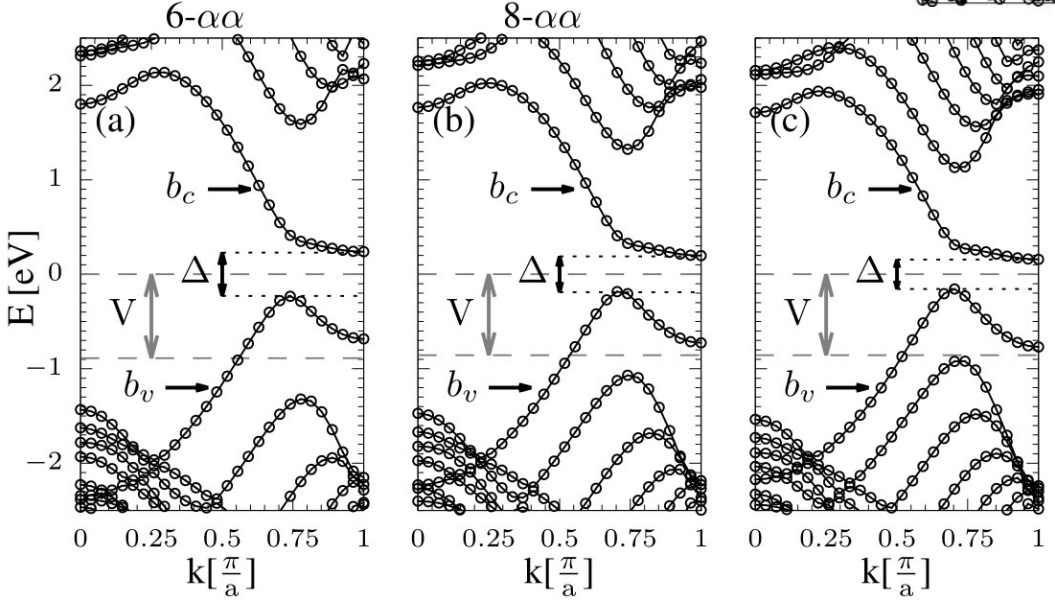


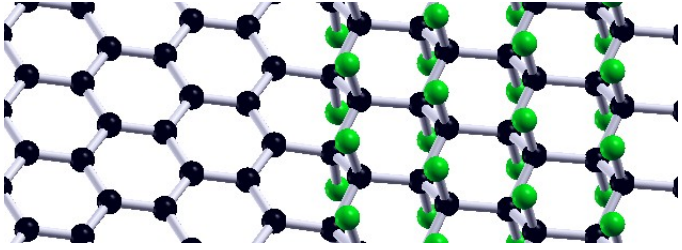
Canales de Grafeno Resultados de primeros principios



Sistema	θ	a_y	M_{abs}	M_α	Δ
6-$\alpha\alpha$	20.5°	25.85Å	$1.10\mu_B$	$0.30\mu_B$	0.47eV
8-$\alpha\alpha$	19.7°	30.09Å	$1.16\mu_B$	$0.30\mu_B$	0.38eV
10-$\alpha\alpha$	18.7°	34.33Å	$1.23\mu_B$	$0.30\mu_B$	0.31eV







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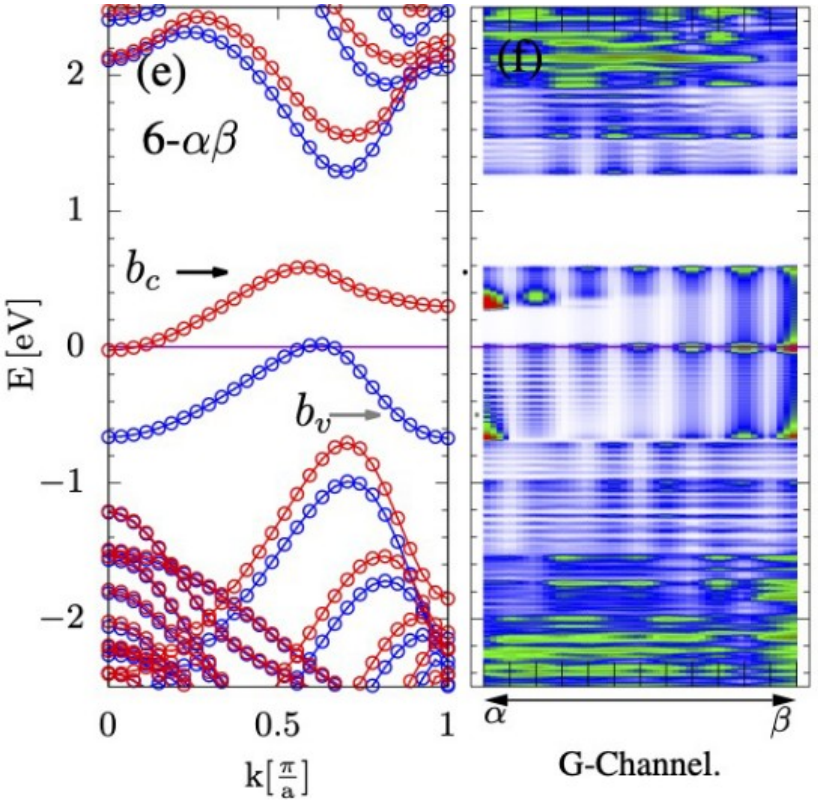
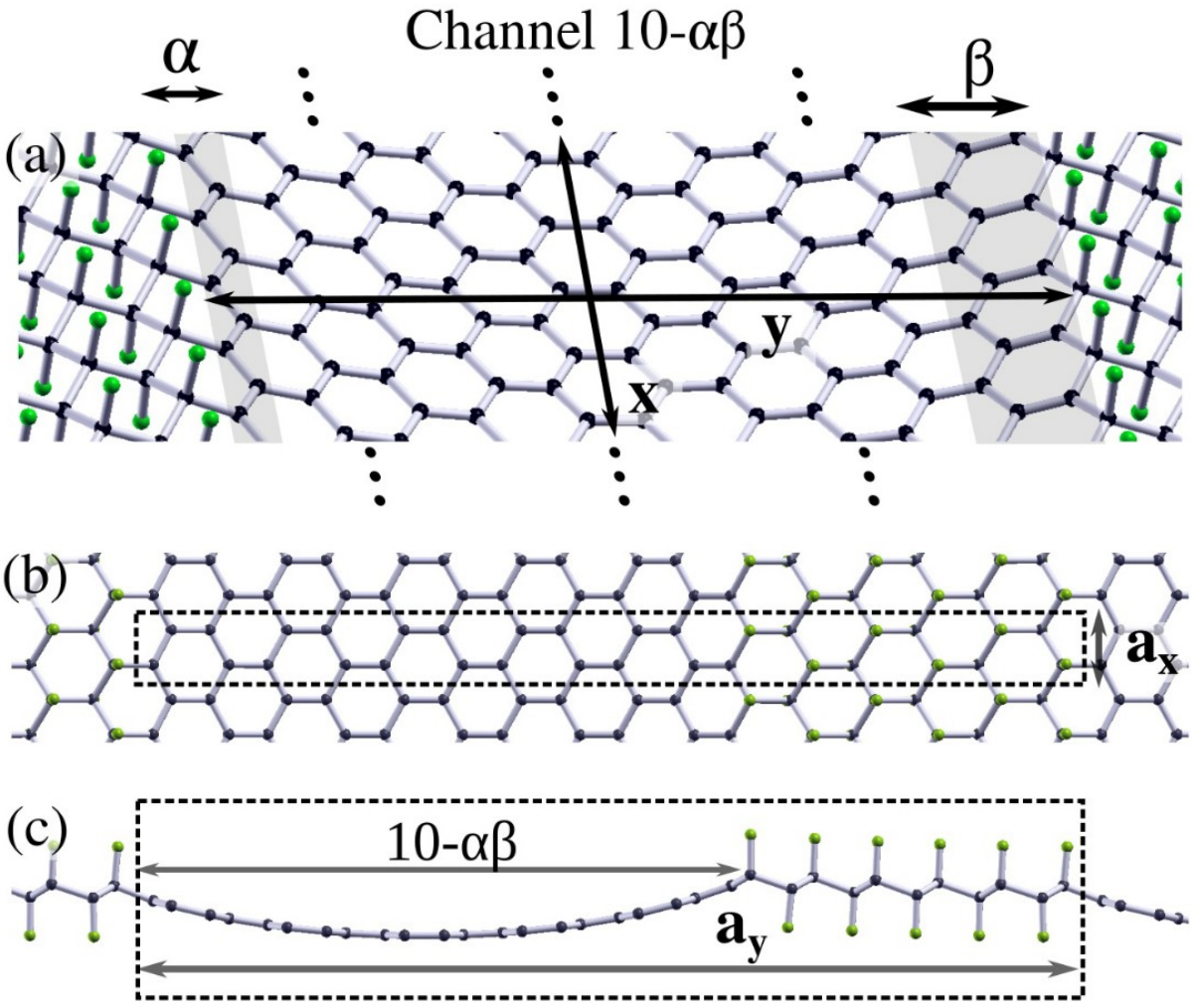
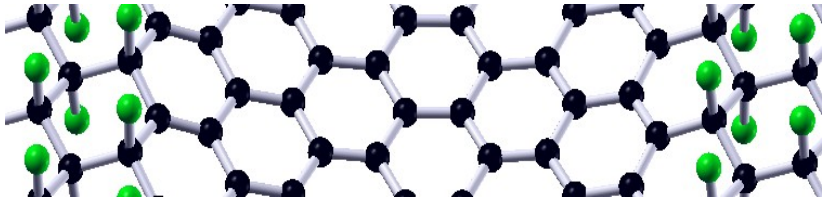
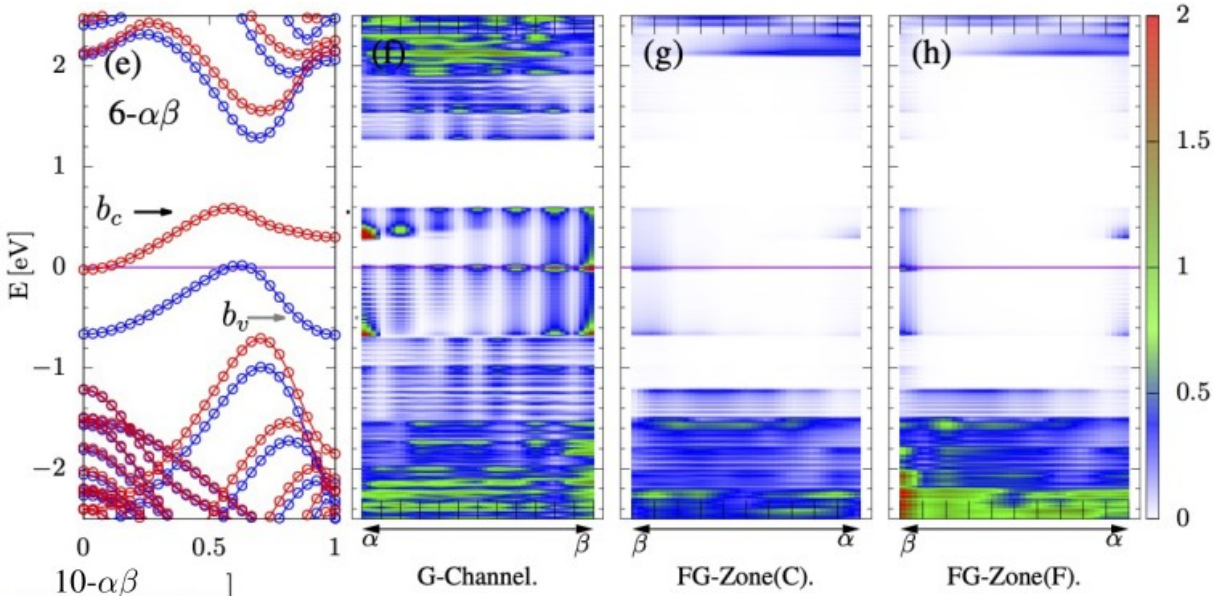
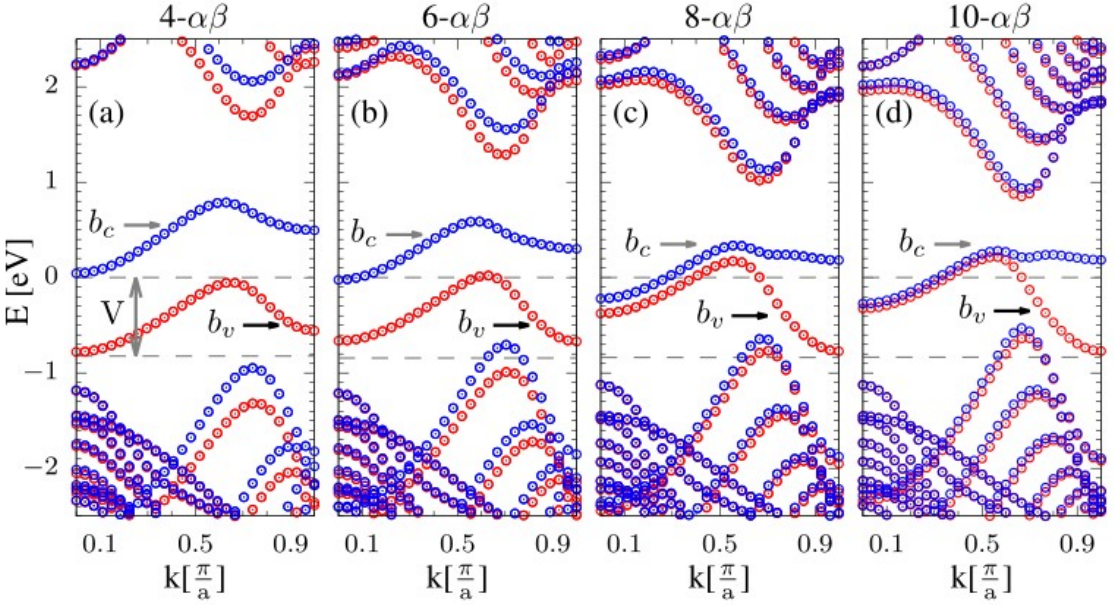


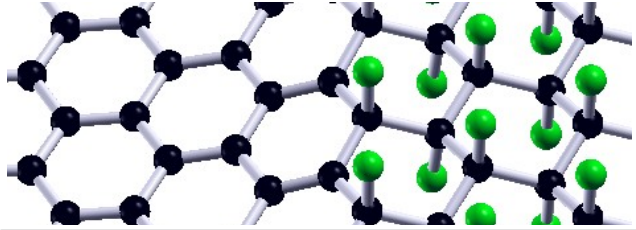


Canales de Grafeno
Resultados de primeros principios





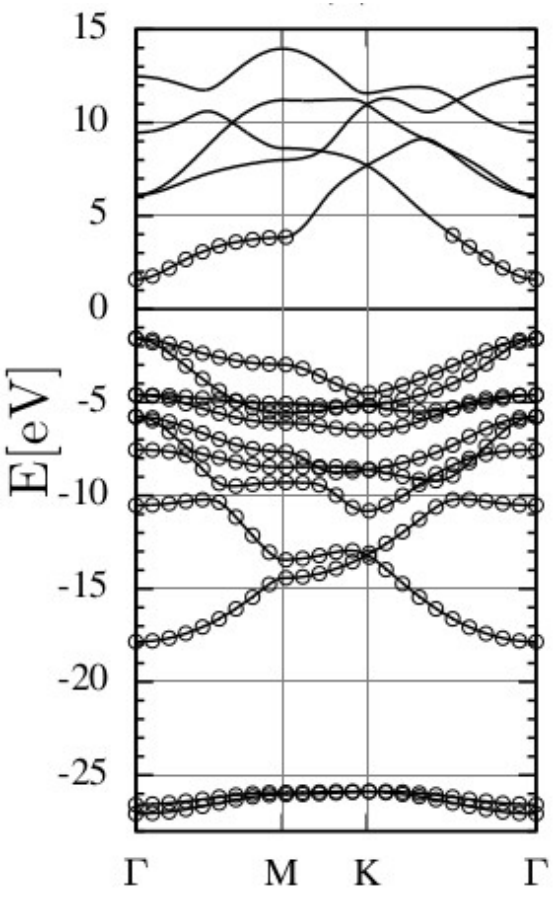




Channel	a_y (Å)	M_{abs} (μ_B)	M_t (μ_B)	M_β (μ_B)	M_α (μ_B)
4-$\alpha\beta$	21.75	1.60	0.97	0.38	0.34
6-$\alpha\beta$	25.83	1.47	0.84	0.31	0.31
8-$\alpha\beta$	30.06	0.82	0.45	0.08	0.31
10-$\alpha\beta$	34.29	0.71	0.37	0.03	0.31

Ajuste de Wannier – Verificación de parámetros.

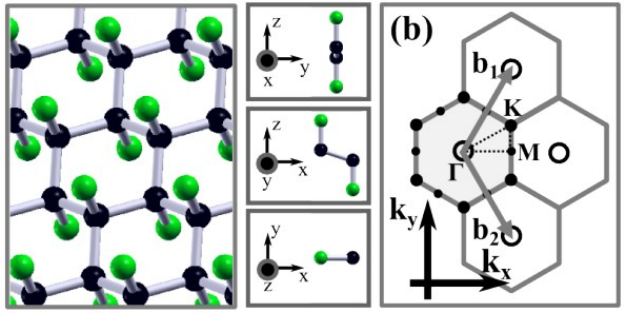
Para un “k” fijo

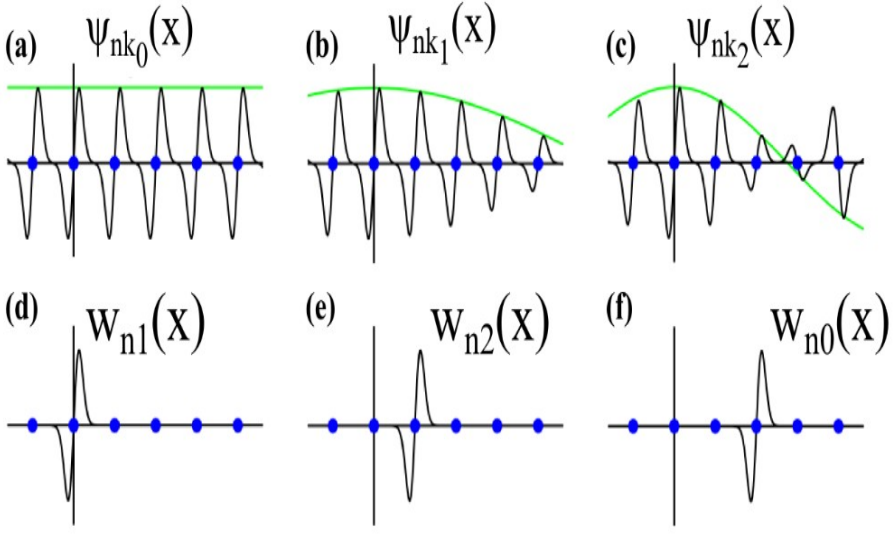


$$\begin{pmatrix} \varepsilon_1 & 0 & 0 & 0 & \cdots \\ 0 & \varepsilon_2 & 0 & 0 & \cdots \\ 0 & 0 & \varepsilon_3 & 0 & \cdots \\ 0 & 0 & 0 & \varepsilon_4 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$|w_{n\mathbf{R}}\rangle = \frac{\Omega}{(2\pi)^3} \int_{ZB} \left[\sum_{m=1} T_{nm}^{(\mathbf{k})} |\psi_{m\mathbf{k}}\rangle \right] e^{i\mathbf{k}\cdot\mathbf{R}}\, d\mathbf{k}$$

$$\mathbf{M}^{(k,b)} = \mathbf{T}^{(\mathbf{k})\dagger} \mathbf{M}^{0,(\mathbf{k},\mathbf{b})} \mathbf{T}^{(\mathbf{k}+\mathbf{b})}$$





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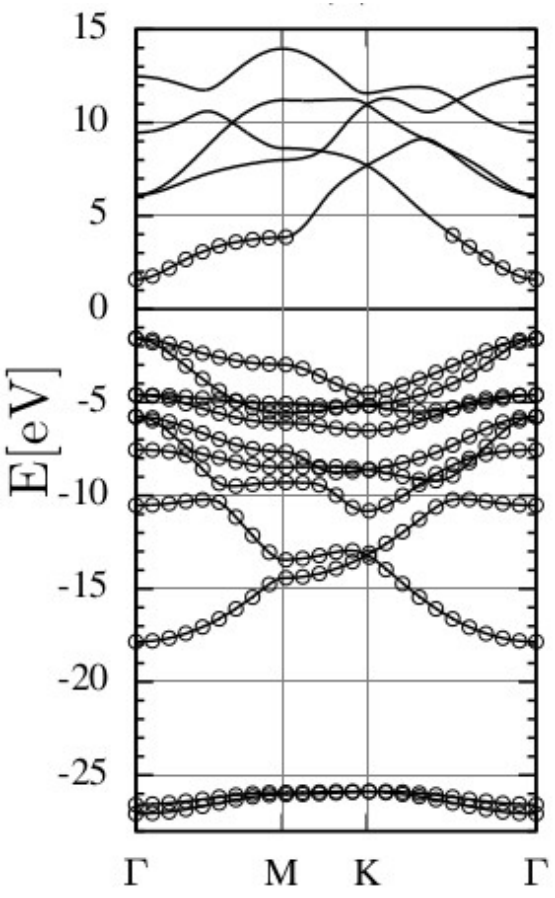
Para un “k” fijo

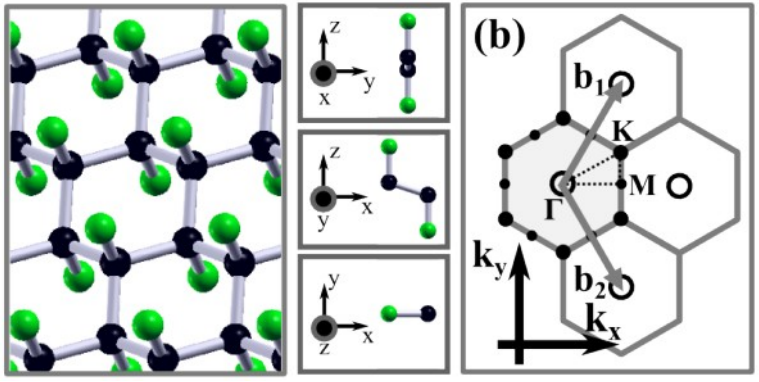


$$\begin{pmatrix} \varepsilon_1 & 0 & 0 & 0 & \cdots \\ 0 & \varepsilon_2 & 0 & 0 & \cdots \\ 0 & 0 & \varepsilon_3 & 0 & \cdots \\ 0 & 0 & 0 & \varepsilon_4 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$|w_{n\mathbf{R}}\rangle = \frac{\Omega}{(2\pi)^3} \int_{ZB} \left[\sum_{m=1} T_{nm}^{(\mathbf{k})} |\psi_{m\mathbf{k}}\rangle \right] e^{i\mathbf{k}\cdot\mathbf{R}}\, d\mathbf{k}$$

$$\mathbf{M}^{(k,b)} = \mathbf{T}^{(\mathbf{k})\dagger} \mathbf{M}^{0,(\mathbf{k},\mathbf{b})} \mathbf{T}^{(\mathbf{k}+\mathbf{b})}$$

$$\mathbf{H} = \begin{pmatrix} \varepsilon_1 & t_{12} & t_{13} & t_{14} & \cdots \\ t_{21} & \varepsilon_2 & t_{23} & t_{24} & \cdots \\ t_{31} & t_{32} & \varepsilon_3 & t_{34} & \cdots \\ t_{41} & t_{42} & t_{43} & \varepsilon_4 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$



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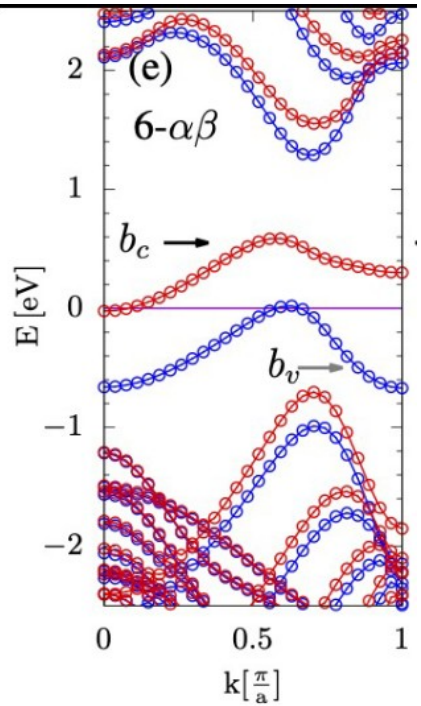
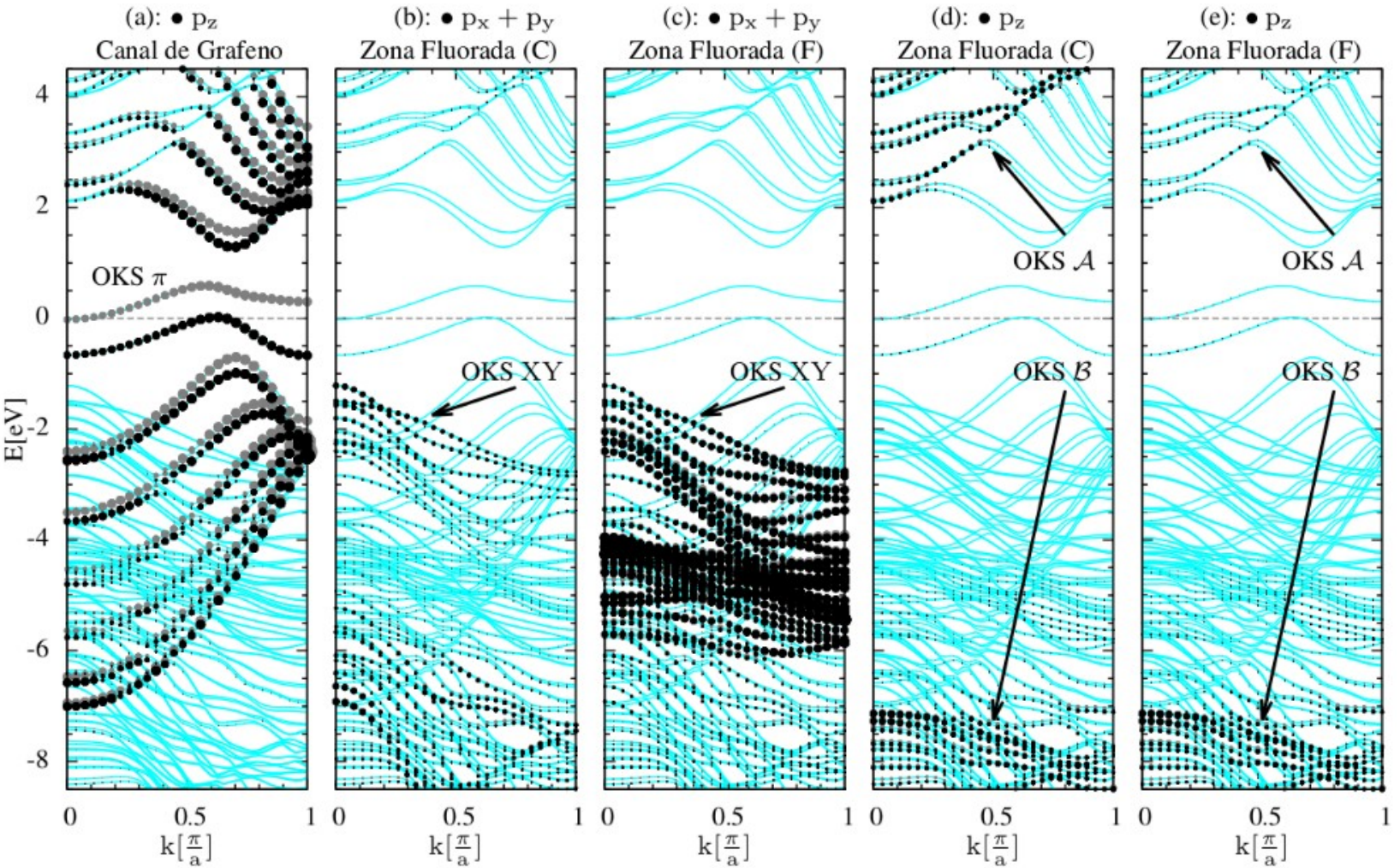
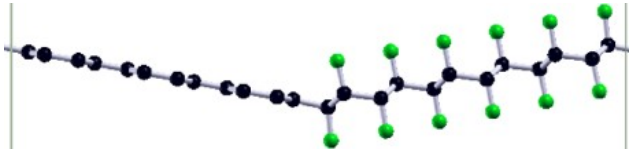
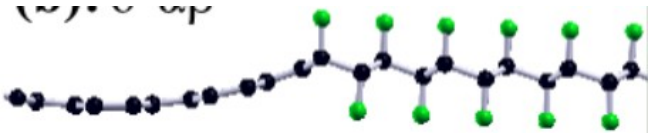
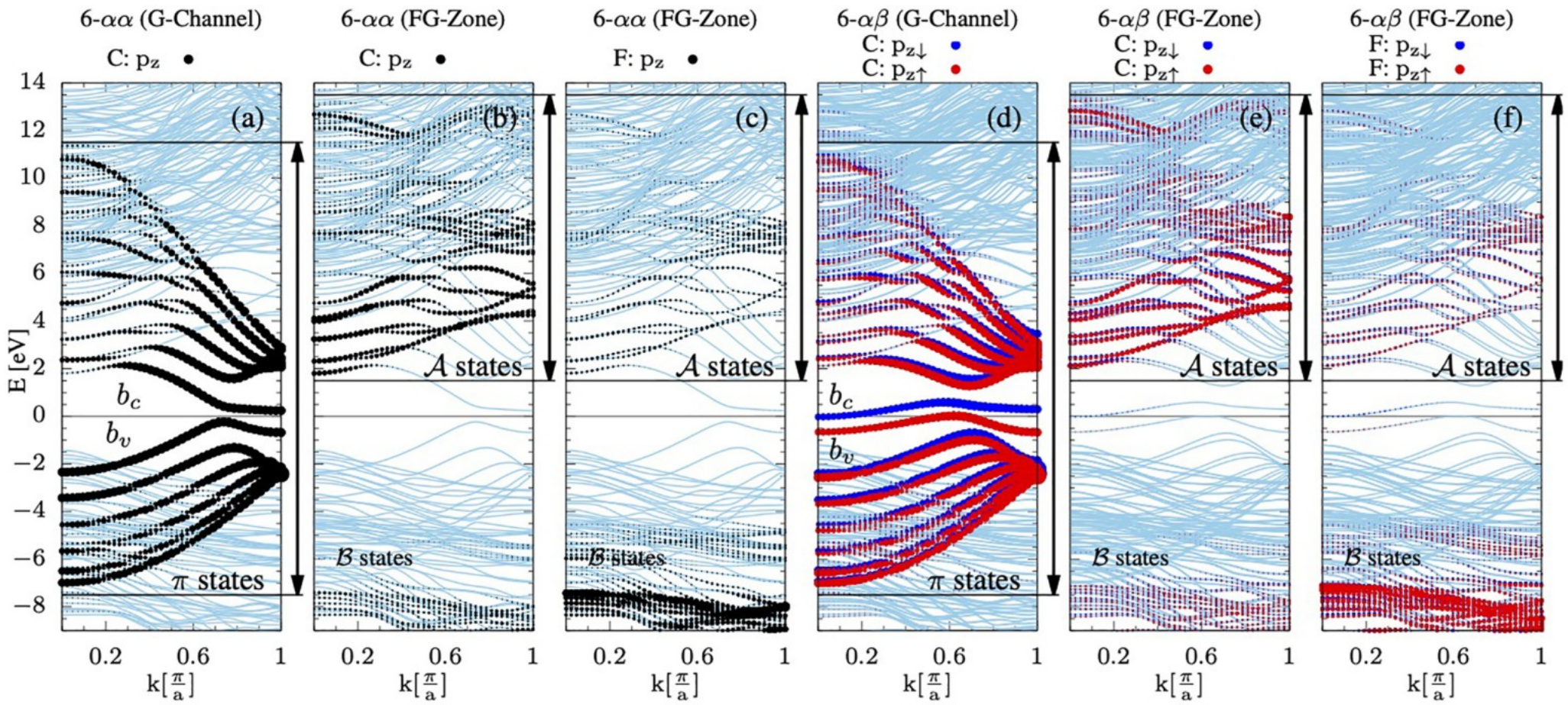




Ajuste de Wannier – Verificación de parámetros.



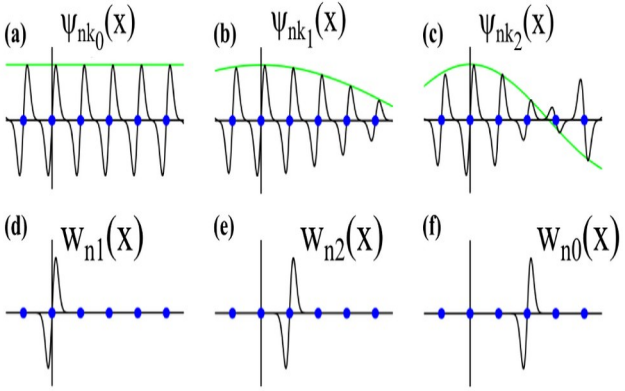


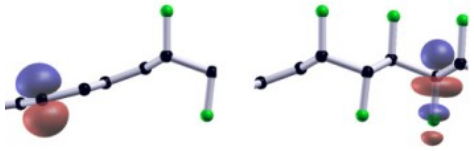


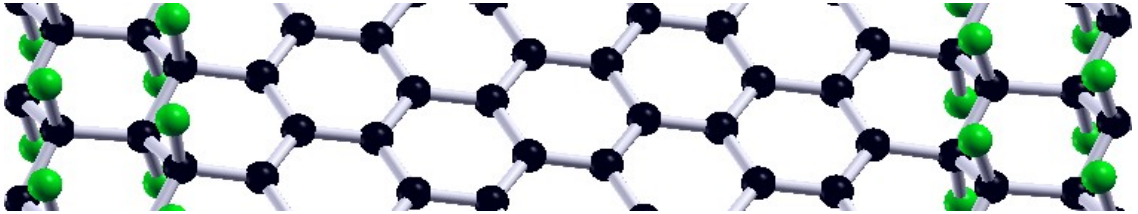
Ajuste de Wannier – Verificación de parámetros.

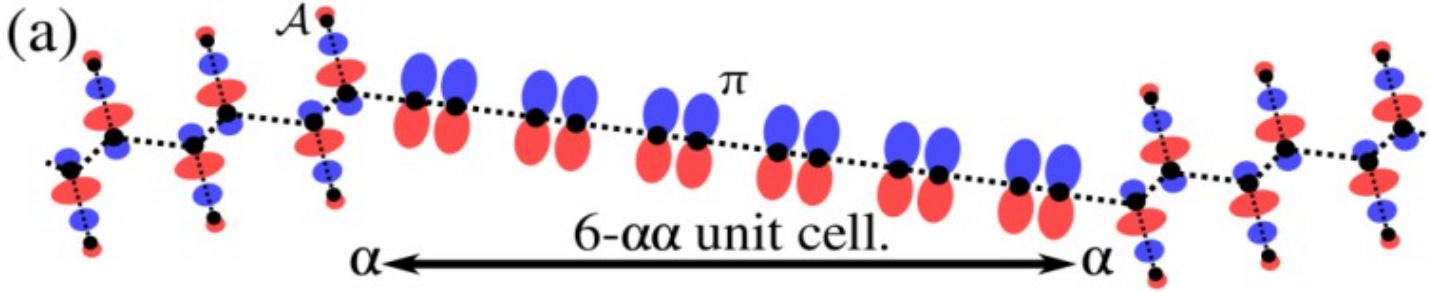
$$|w_{n\mathbf{R}}\rangle = \frac{\Omega}{(2\pi)^3}\int_{ZB}\left[\sum_{m=1} T_{nm}^{(\mathbf{k})}\,|\psi_{m\mathbf{k}}\rangle\right] e^{i\mathbf{k}\cdot\mathbf{R}}\,d\mathbf{k}$$

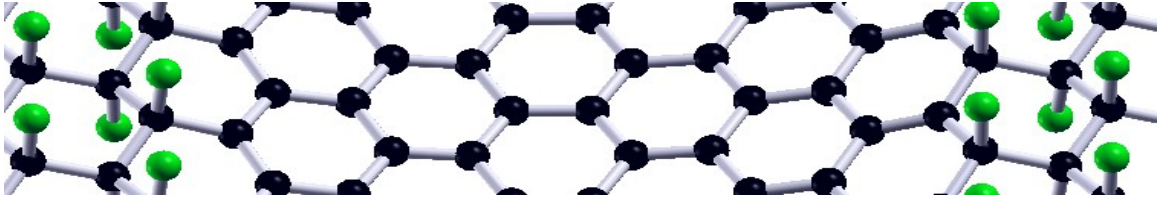
$$\mathbf{M}^{(k,b)} = \mathbf{T}^{(\mathbf{k})\dagger}\mathbf{M}^{0,(\mathbf{k},\mathbf{b})}\mathbf{T}^{(\mathbf{k}+\mathbf{b})}$$

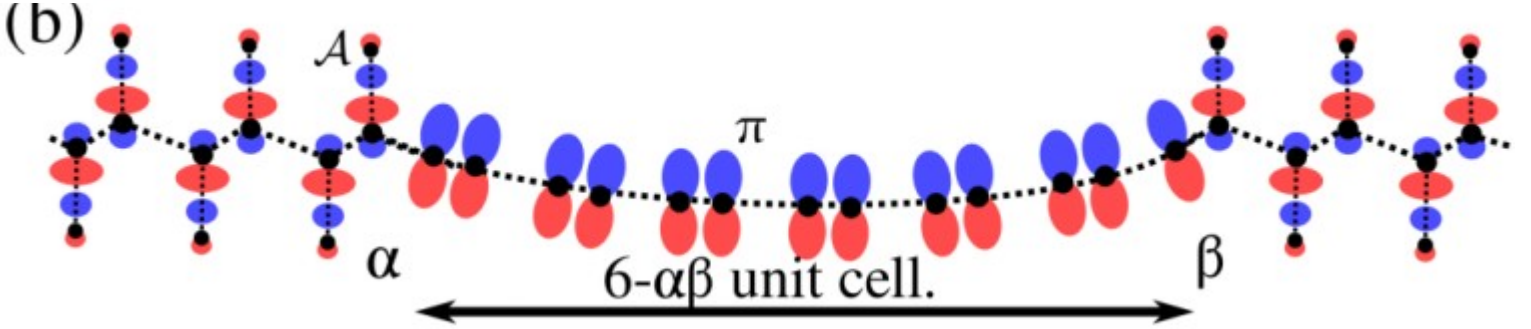




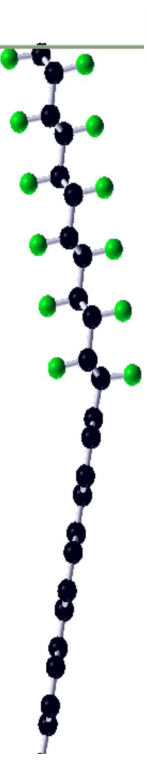


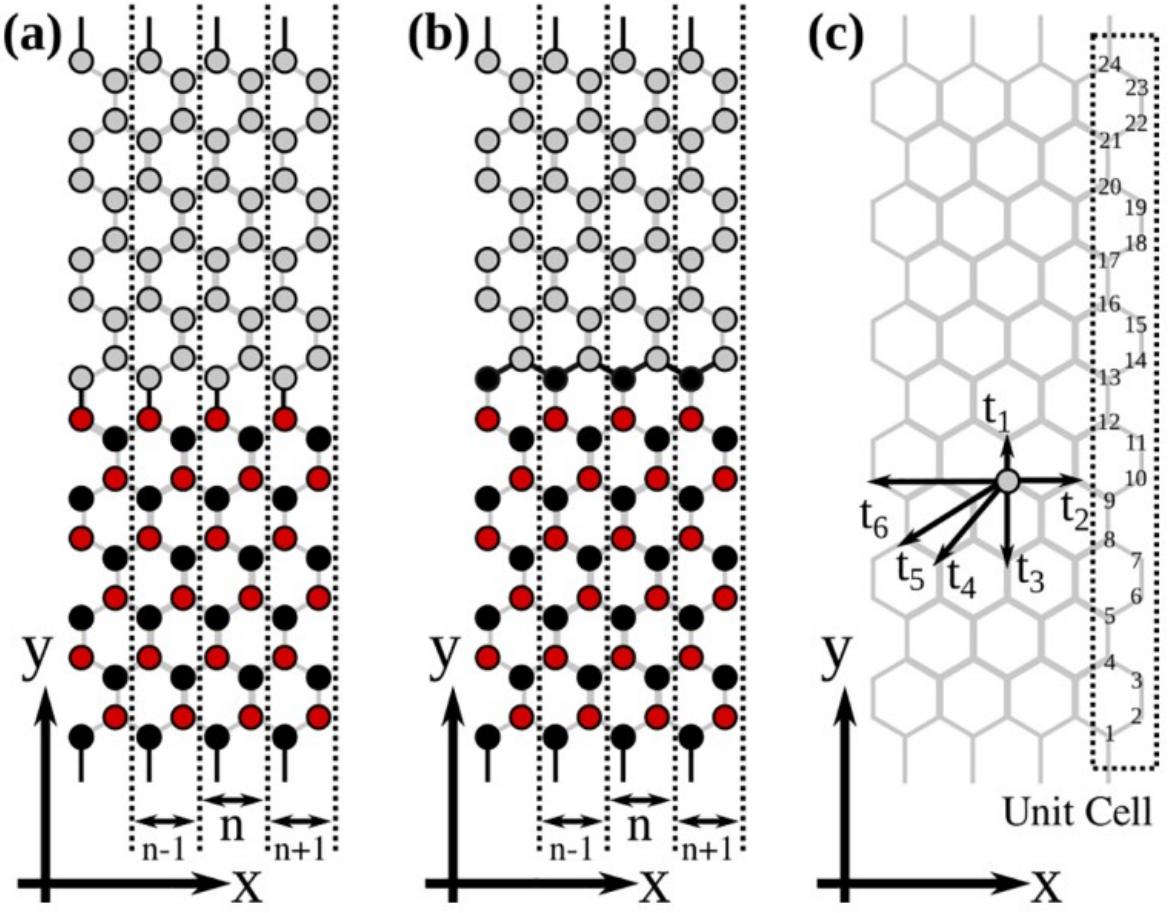






Modelo de Hubbard y método Hartree-Fock





$$U_j = -\frac{\varepsilon_{j\uparrow} - \varepsilon_{j\downarrow}}{\langle \hat{n}_{j\uparrow} \rangle - \langle \hat{n}_{j\downarrow} \rangle} = -\frac{\Delta\varepsilon_{j\sigma}}{\langle \hat{m}_j \rangle}$$

Funciones de Bloch

$$\mathbf{H} = \begin{pmatrix} \varepsilon_1 & 0 & 0 & 0 & \cdots \\ 0 & \varepsilon_2 & 0 & 0 & \cdots \\ 0 & 0 & \varepsilon_3 & 0 & \cdots \\ 0 & 0 & 0 & \varepsilon_4 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

Funciones de Wannier

$$\mathbf{H} = \begin{pmatrix} \varepsilon_1 & t_{12} & t_{13} & t_{14} & \cdots \\ t_{21} & \varepsilon_2 & t_{23} & t_{24} & \cdots \\ t_{31} & t_{32} & \varepsilon_3 & t_{34} & \cdots \\ t_{41} & t_{42} & t_{43} & \varepsilon_4 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$H_{AH} = \sum_{j,\sigma} \varepsilon_j \, c^{\dagger}_{j\sigma} \, c_{j\sigma} - \sum_{j,l,\sigma} t_{jl} \, c^{\dagger}_{j\sigma} c_{l\sigma} + \sum_{j} U_j \, \hat{n}_{j\uparrow} \, \hat{n}_{j\downarrow}$$

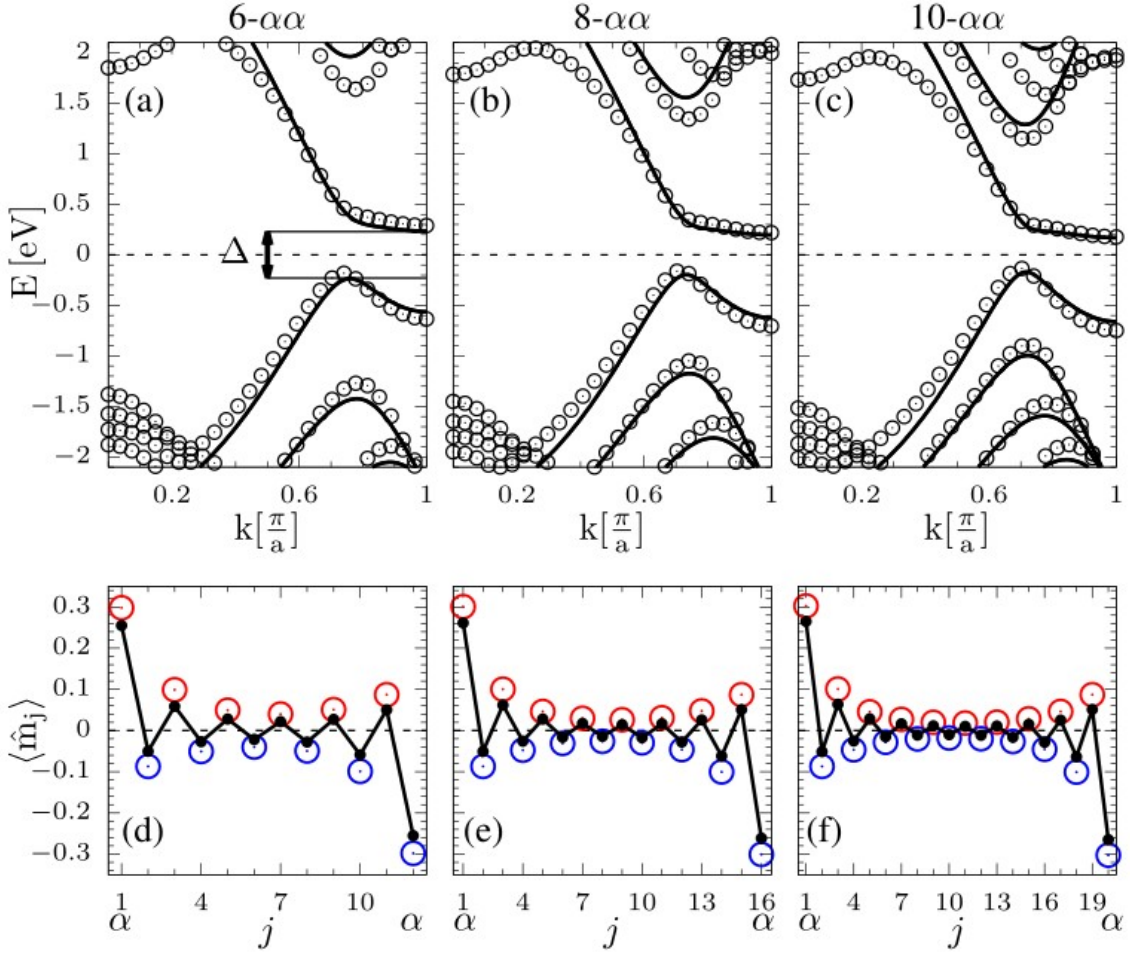
Hartree - Fock

$$\bar{H}_{AH} = \sum_{j,\sigma} \varepsilon_{j\sigma} \, c^{\dagger}_{j\sigma} c_{j\sigma} - \sum_{j,l,\sigma} t_{jl} \, c^{\dagger}_{j\sigma} c_{l\sigma}$$

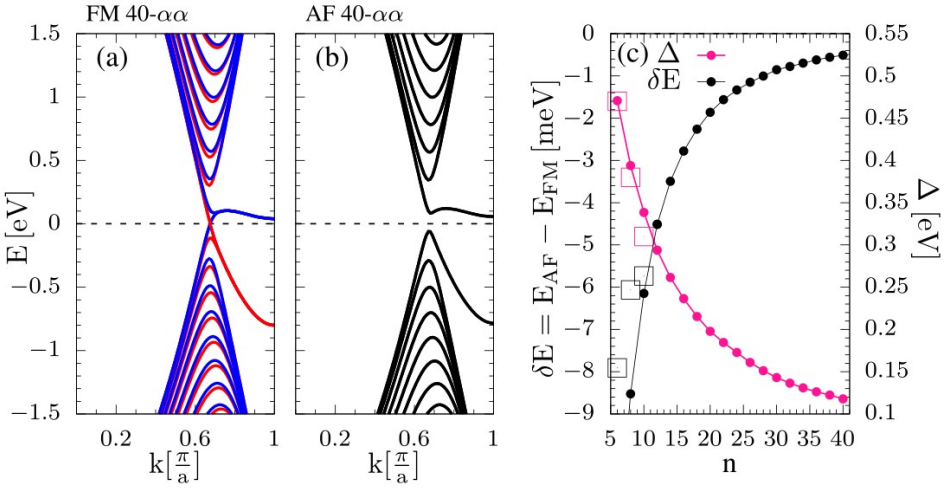
$$\varepsilon_{j\uparrow} = \varepsilon_j + U_j \langle \hat{n}_{j\downarrow} \rangle ,$$

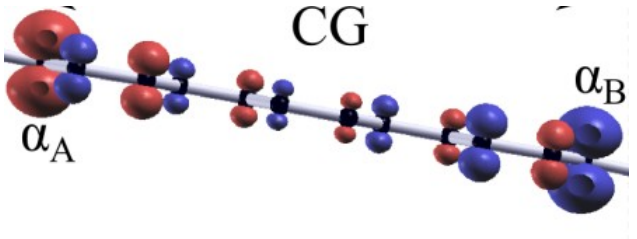
$$\varepsilon_{j\downarrow} = \varepsilon_j + U_j \langle \hat{n}_{j\uparrow} \rangle .$$

Ajuste de los resultados DFT.

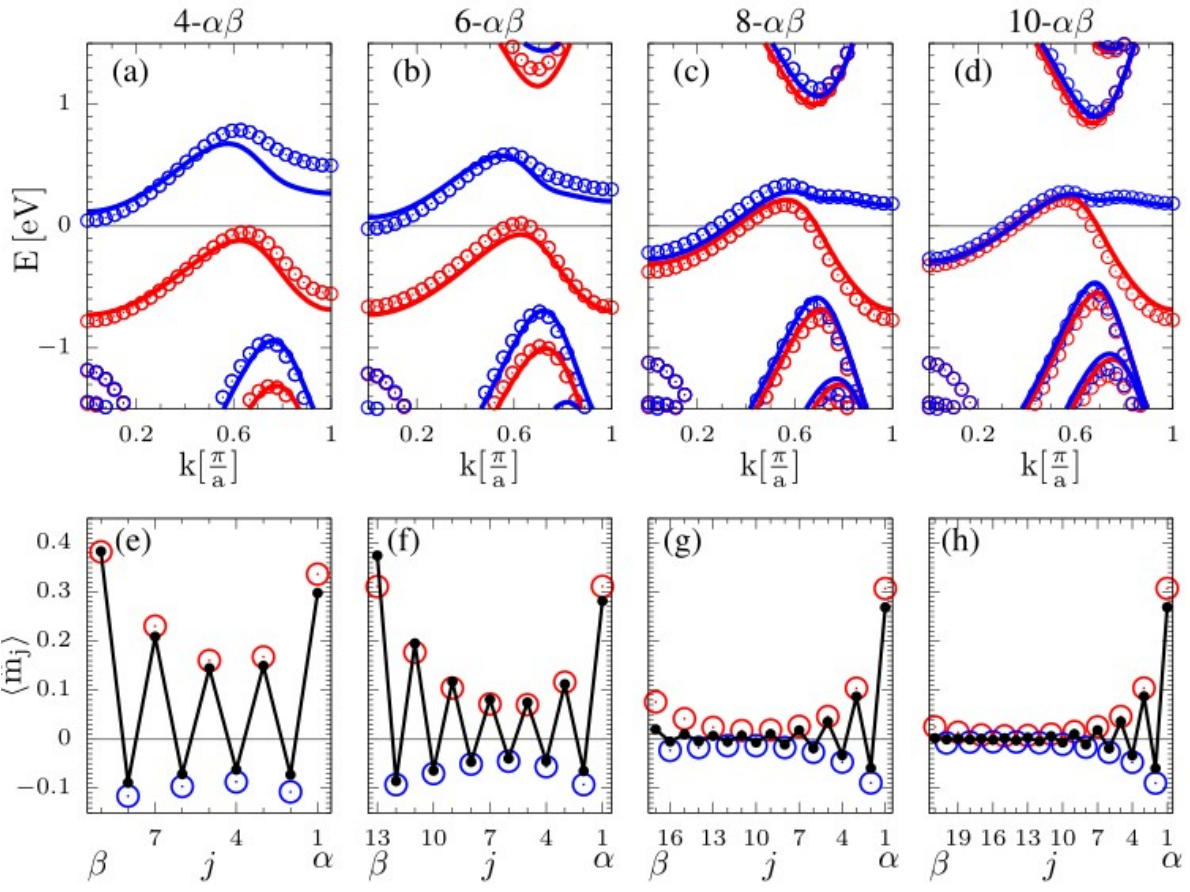


Predicción

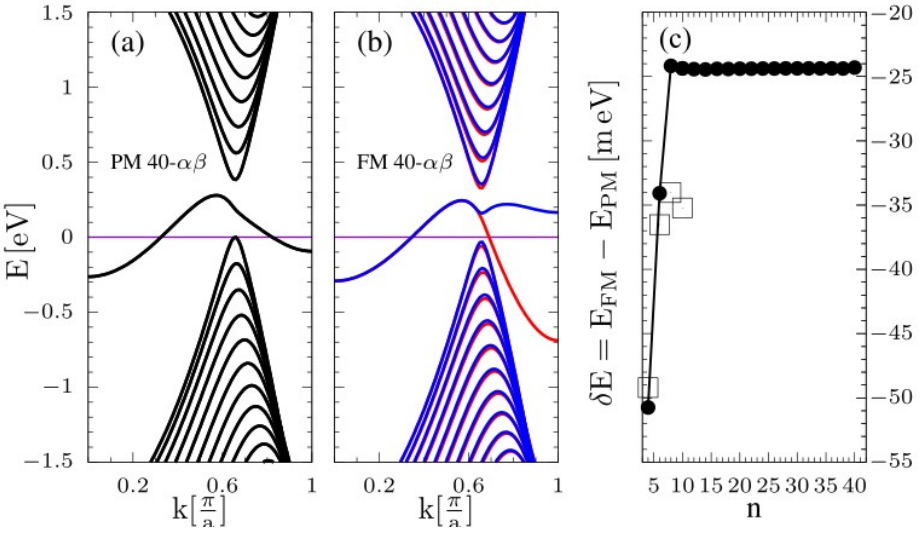


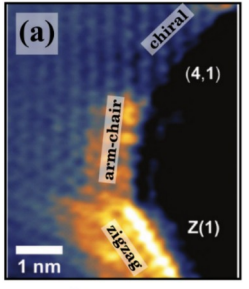


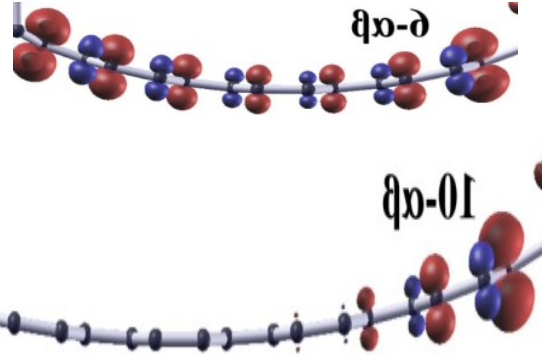
Ajuste de los resultados DFT.



Predicción







Conclusiones – Referencias.

1. Los canales de grafeno (F-GNR) tienen propiedades similares a las cintas de grafeno (ZGNR).
2. La diferencia entre estados de borde F-GNR respecto las ZGNR es su localización, que permite sintonizar un cambio de fase respecto el ancho del canal.
3 Los orbitales de Wannier reproducen los resultados DFT de sistemas con enlaces covalentes.

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Electronic and magnetic properties of graphene-fluorographene nanoribbons: Controllable semiconductor-metal transition

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