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¿Son los derivados de grafeno el futuro de este material?

Lunes, 12 de marzo, 13:00 h.
Aula III (edificio Trilingüe)

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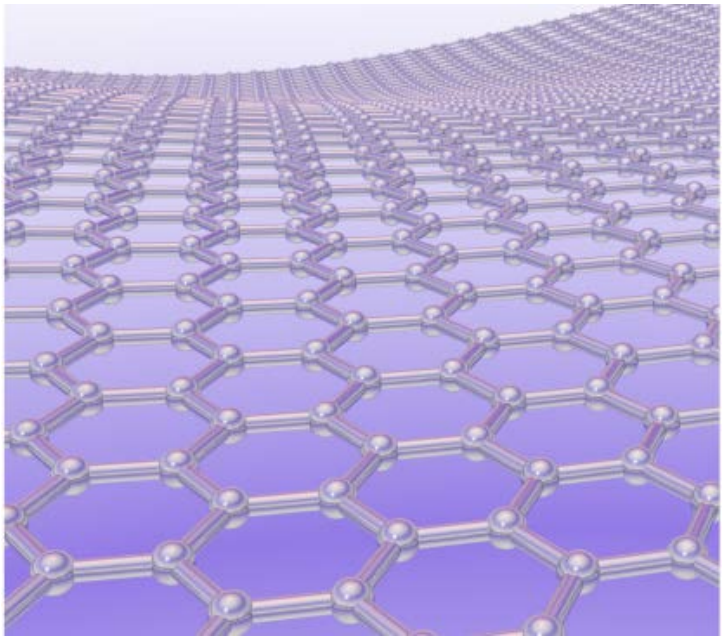
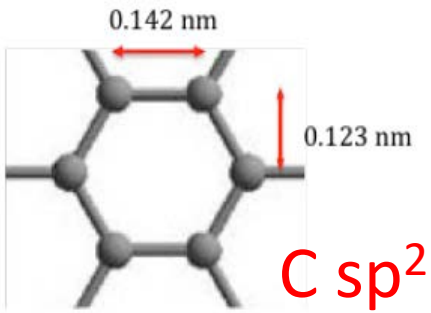
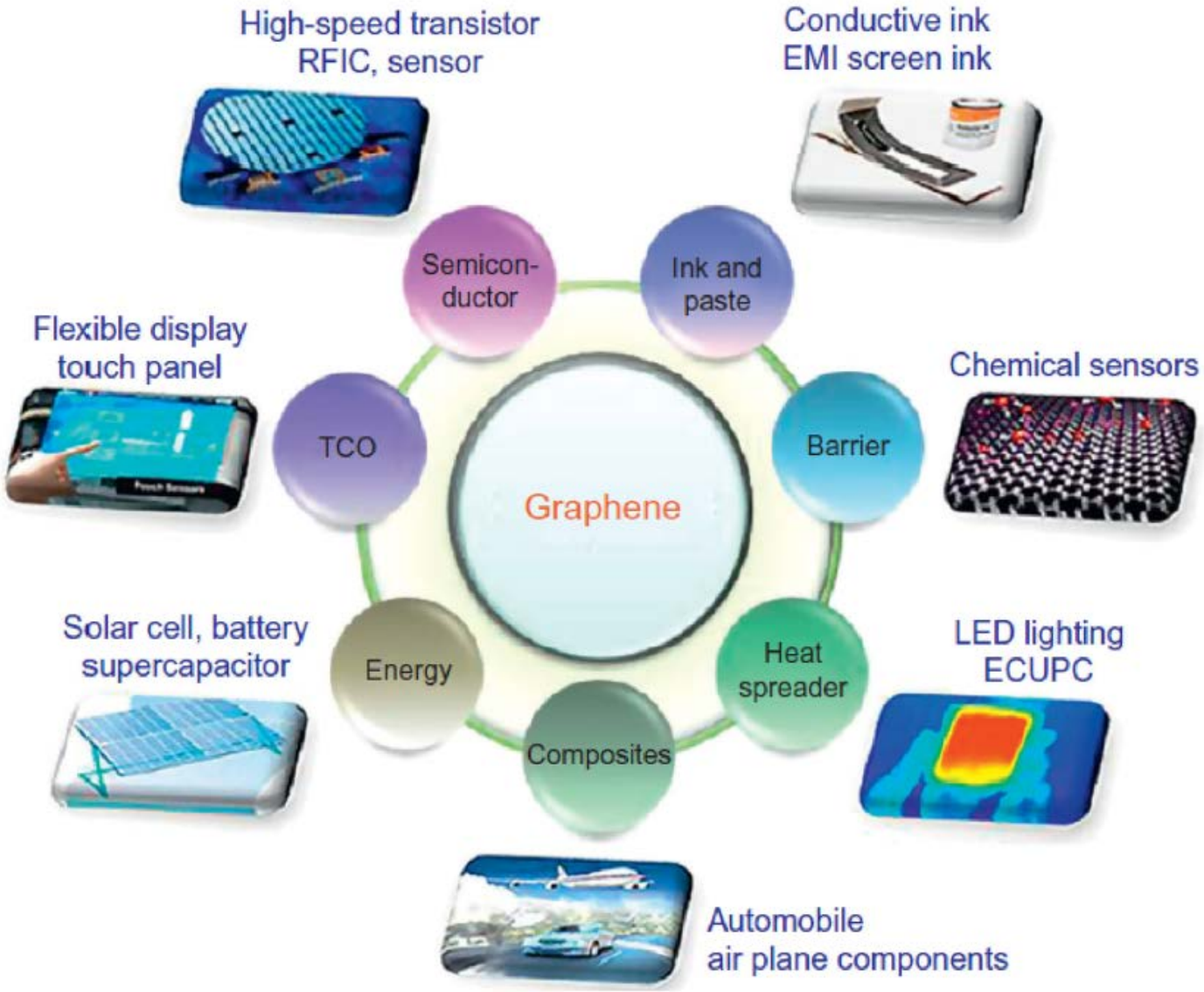
Unidad de Excelencia de Nanoelectrónica y Nanomateriales de la Universidad de Salamanca, USAL-NANOLAB

Grafeno

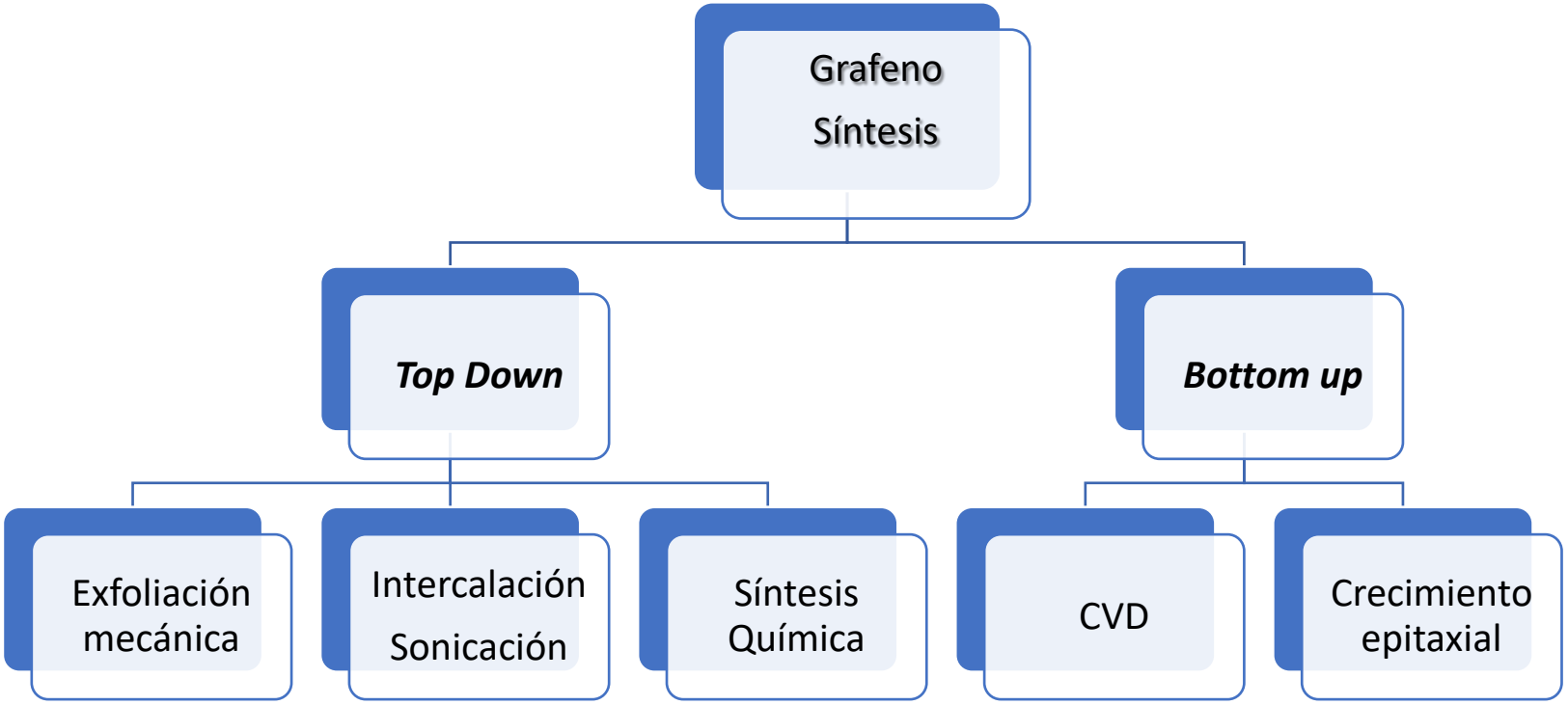




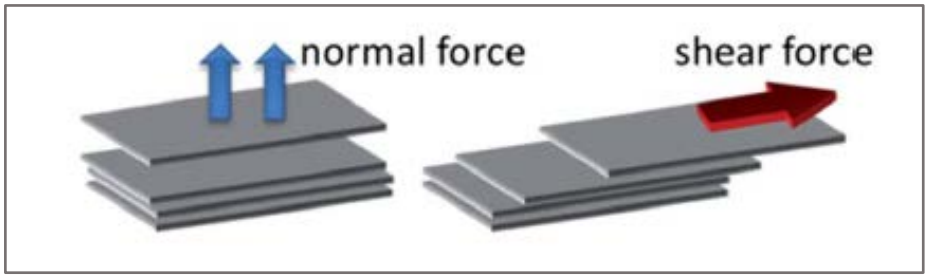
- ✓ baja densidad, 0.79 mg/m^2
- ✓ transparencia (absorción 2.3%)
- ✓ alta resistencia mecánica , 200 veces acero
- ✓ alta conductividad eléctrica, 100 veces silicio
- ✓ alto módulo de Young, ~ 1 TPa

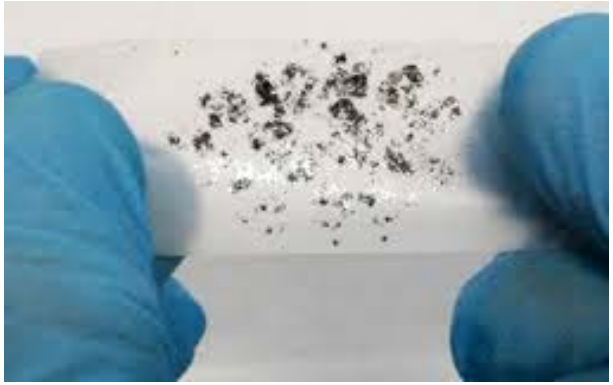

High-speed transistor
RFIC, sensor
Conductive ink
EMI screen ink
Semicon-
ductor
Ink and
paste
Flexible display
touch panel
Chemical sensors
TCO
Graphene
Barrier
Solar cell, battery
supercapacitor
Energy
Heat
spreader
LED lighting
ECUPC
Composites
Automobile
air plane components

Obtención de Grafeno

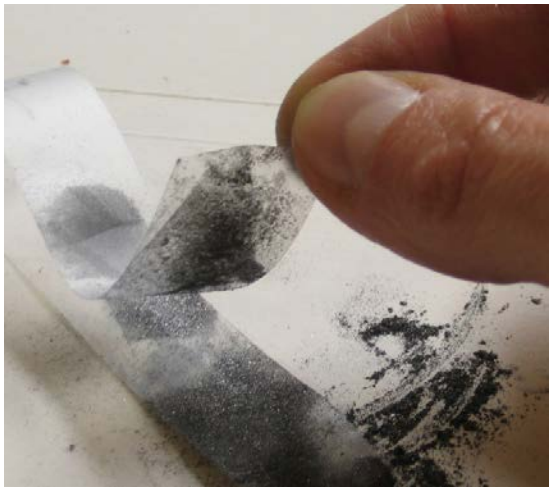


Exfoliación micromecánica

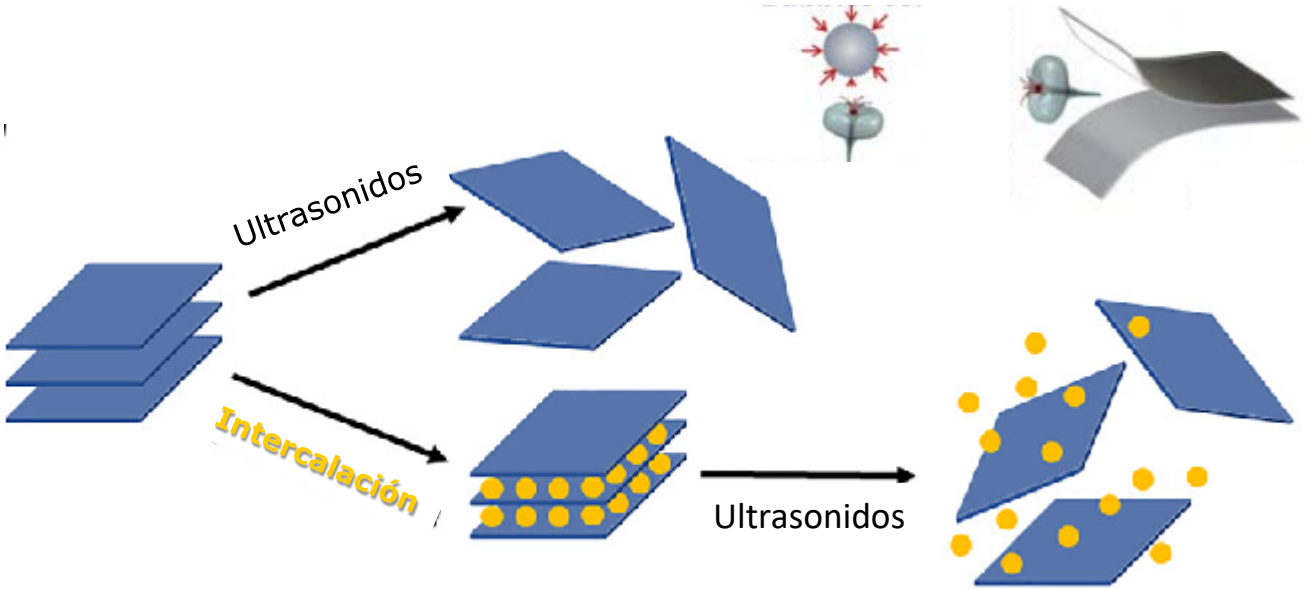




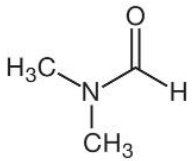
Grafeno de alta calidad



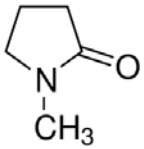
Exfoliación por intercalación y Ultrasonidos



$$\frac{\Delta H_{mix}}{V_{mix}} \approx \frac{2}{T_{flake}}(\delta_G - \delta_{sol})^2 \phi$$

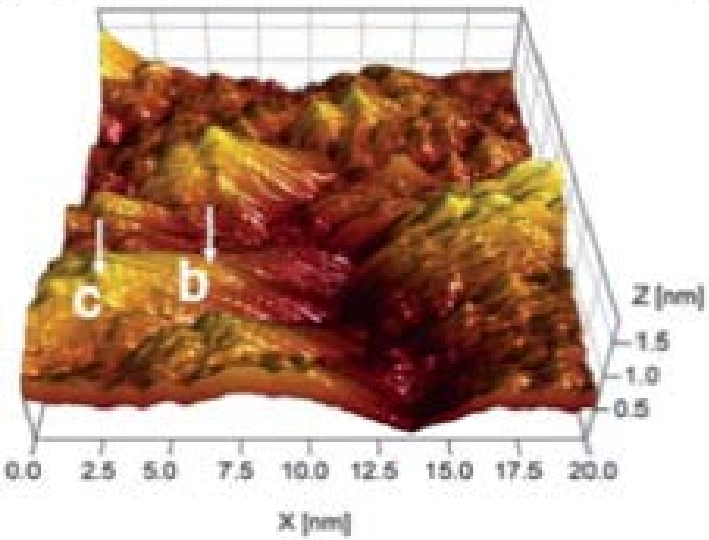


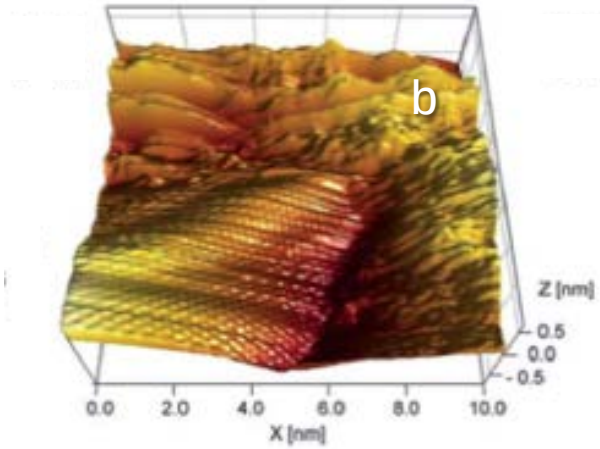
Dimetil formamida

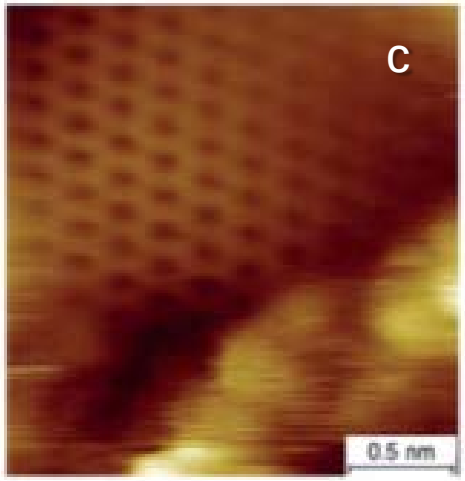


Metil Pirrolidona

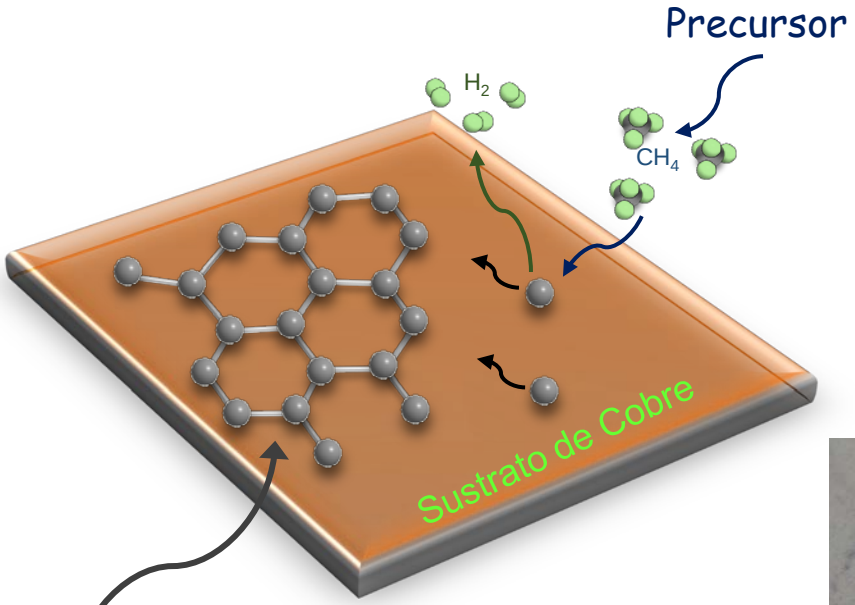
Exfoliación por intercalación y Ultrasonidos



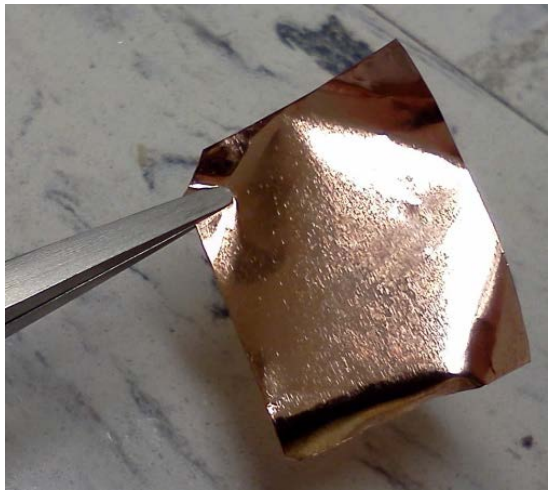




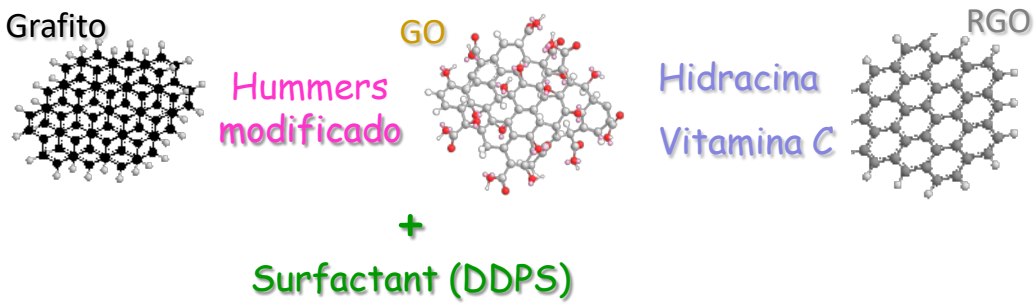
Deposición Química de Vapor (CVD)



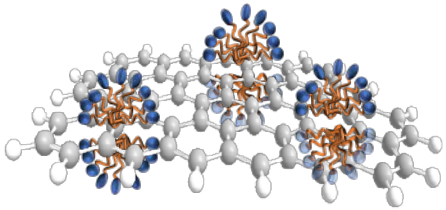
Grafeno policristalino

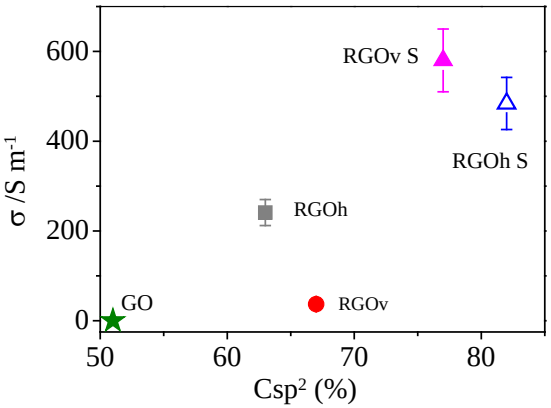


Exfoliación Química



Sample	λ_{max} / nm	% C (sp^2)	I_D/I_G	Conductivity / S m^{-1}
Graphite Oxide	230 ± 2	49 ± 1		Insulator
RGO Hydrazine	264 ± 2	63 ± 2	---	241 ± 29
RGO Hydrazine (DDPS)	268 ± 2	82 ± 1	1.45	484 ± 58
RGO Vitamin C	265 ± 2	67 ± 1	0.67	37 ± 4
RGO Vitamin C (DDPS)	266 ± 2	77 ± 6	0.92	580 ± 70





REDUCCIÓN NO RESTAURA LA ESTRUCTURA DEL GRAFENO

Velázquez et al. *ChemPhysChem* 13, 3682, **2012**
Velázquez et al. *Two-dimensional Materials*, Chap. 2, **2016**

Derivados de grafeno: GO

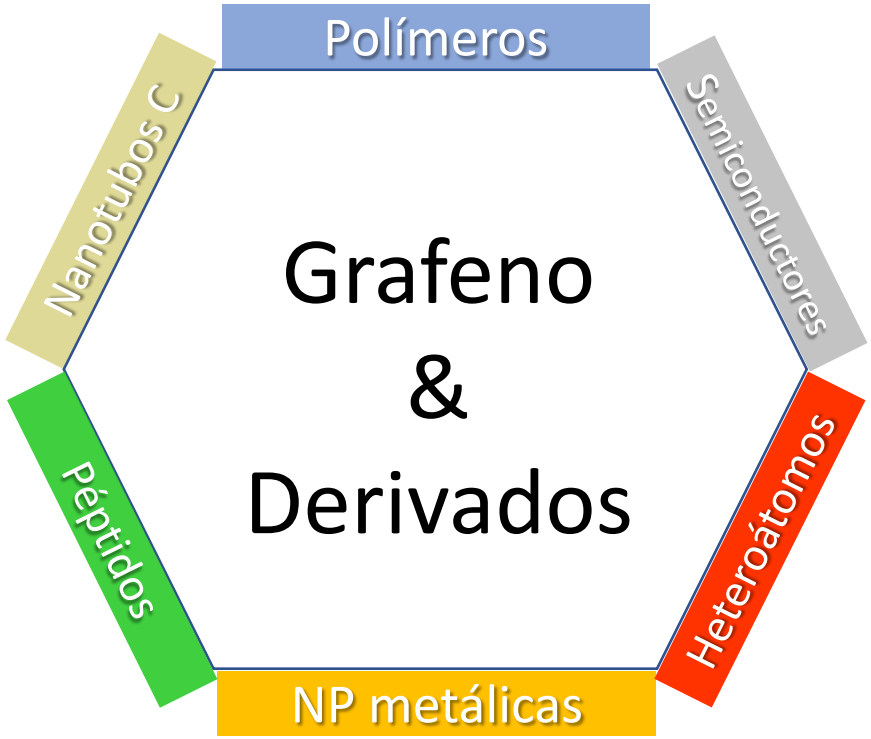
Desventaja:

Los grupos Oxigenados modifican las propiedades del grafeno

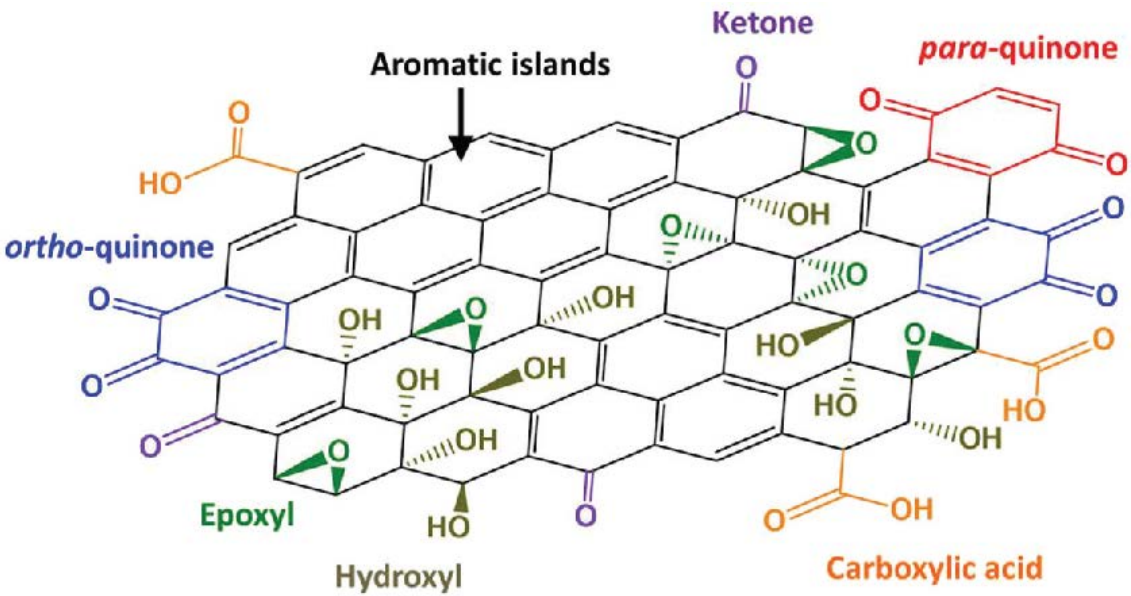
Ventajas:

- Los grupos Oxigenados permiten UNIR POLÍMEROS, NANOPARTÍCULAS, MOLÉCULAS que permiten modular las propiedades del nanomaterial
- Se dispersan fácilmente en agua

Derivados de grafeno: materiales híbridos



¿Cuál es la estructura del GO?

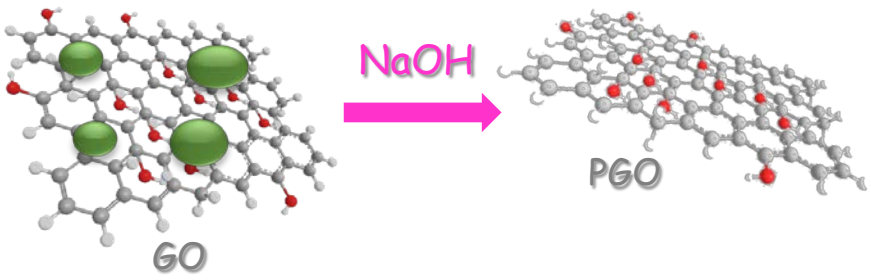


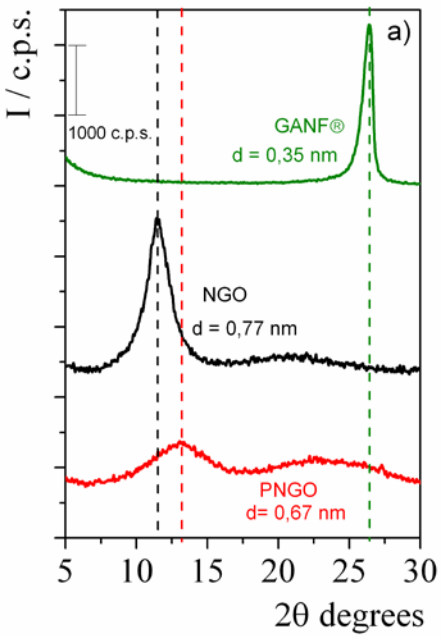
- Hay acuerdo en el tipo de grupos funcionales
- Grandes discrepancias en la proporción

Óxido de grafeno: estructura

Composición química depende de:

- Reacción utilizada para la oxidación
- Material de Partida usado en la oxidación
- Proceso de Reducción: químico o térmico
- Proceso de Purificación

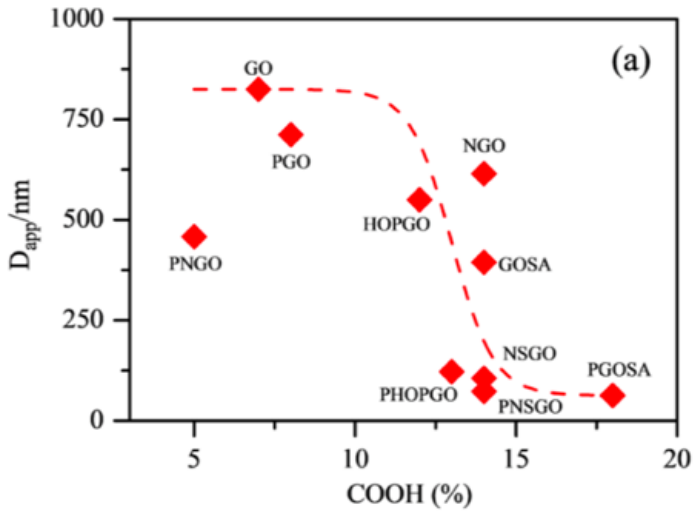




Velázquez et al. *ChemPhysChem* 14, 4002, **2013**
Velázquez et al. *Langmuir* 31, 2697, **2015**
Velázquez et al. *Two-dimensional Materials*, Chap. 2, **2016**

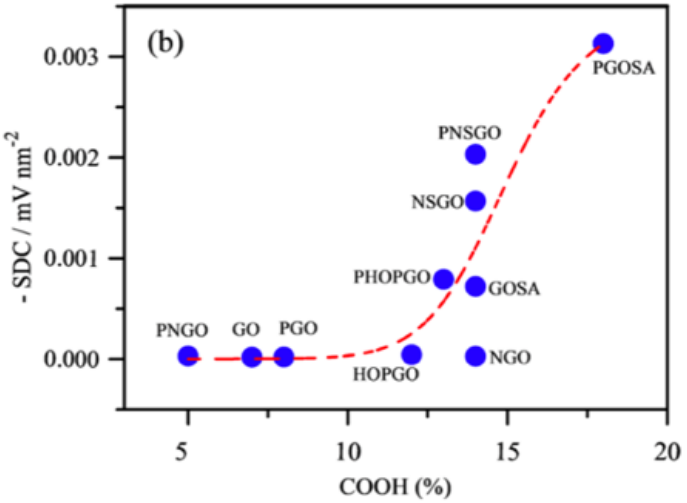
Óxido de grafeno: estructura

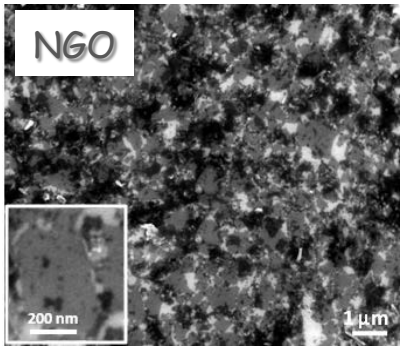
Composición química influye en:



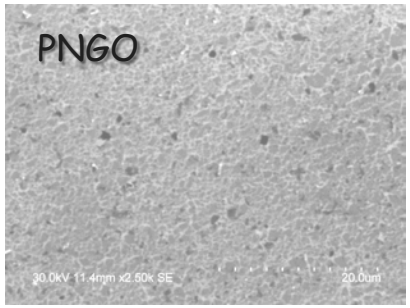
Tamaño de las plaquetas: DLS y FESEM

Densidad de Carga: potencial ζ





Recubrimiento

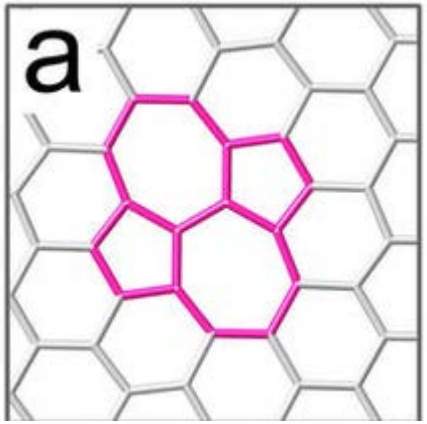


Tipo de defectos

Velázquez et al. *Langmuir* 31, 2697, **2015**

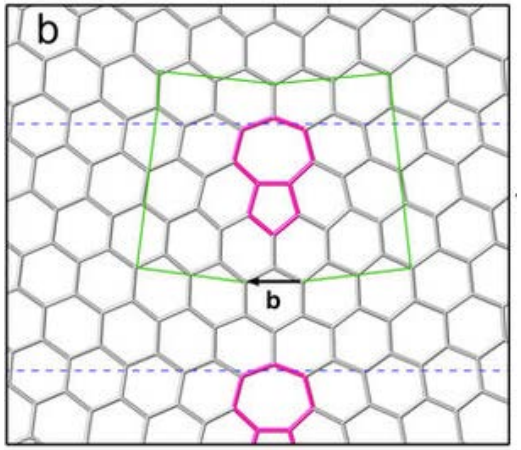
¿Qué entendemos como defectos?

Stone -Wales



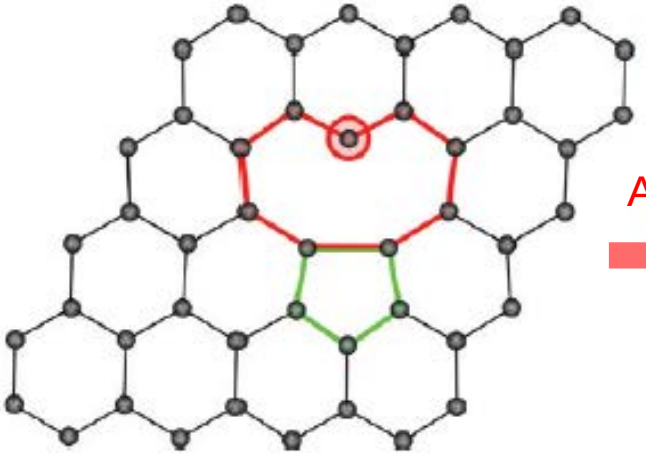
Se repite periódicamente

Grain boundary

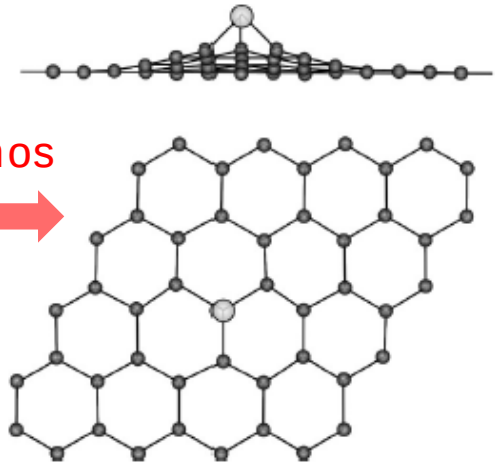


ej. Grafeno CVD

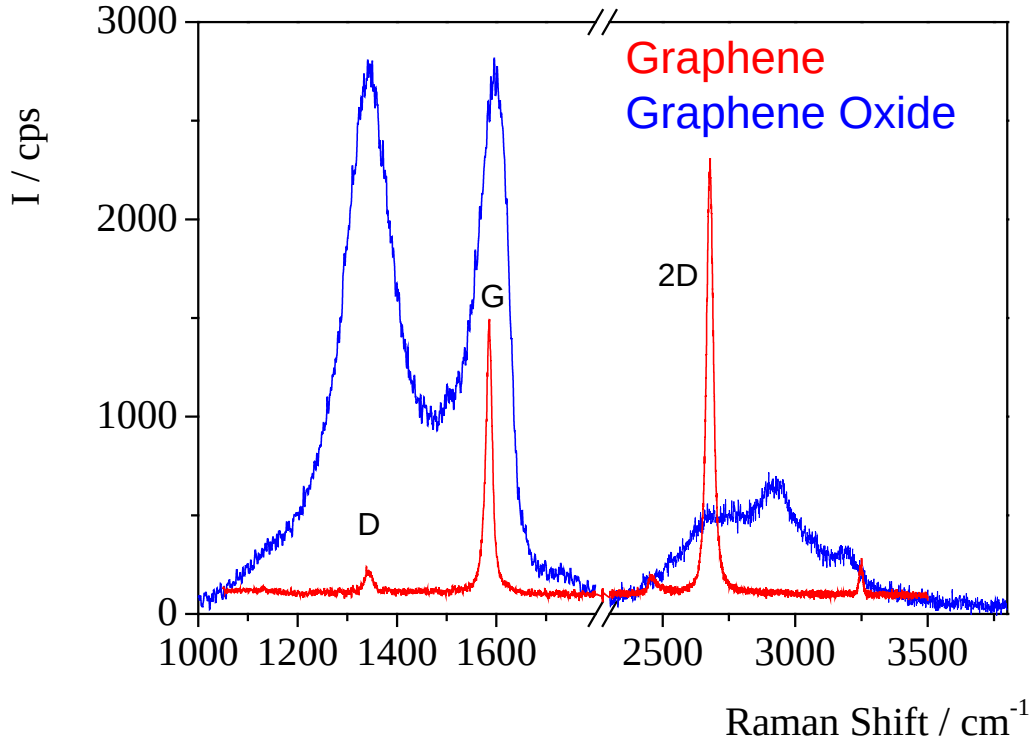
Vacantes



Adsorción de átomos



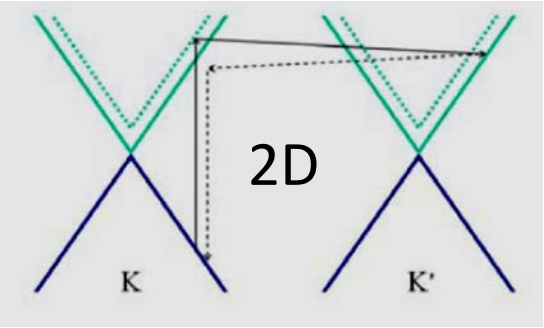
Óxido de grafeno: defectos estructurales



Efecto Raman

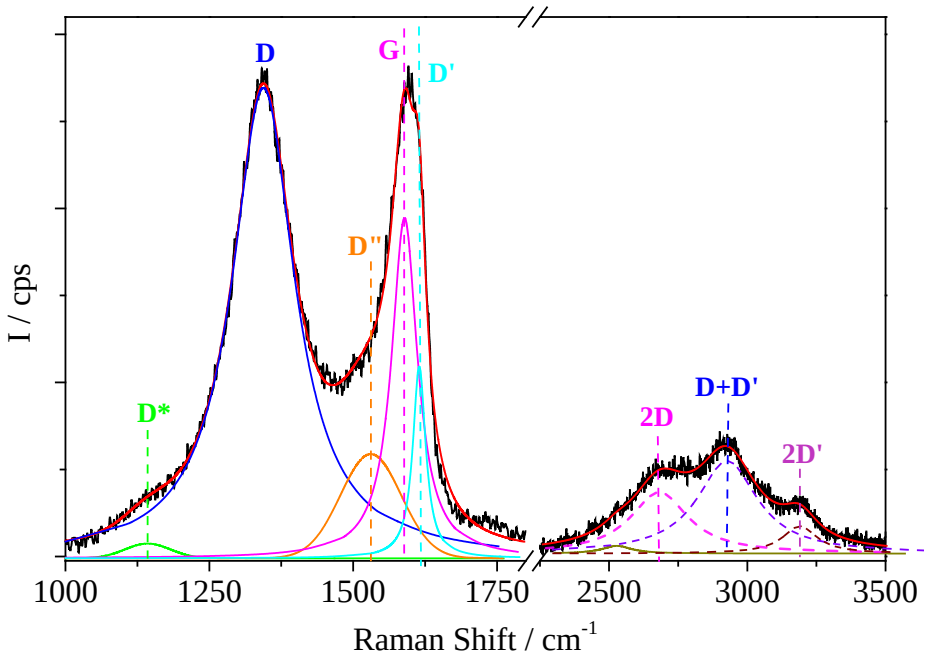
Banda G

Doble Resonancia



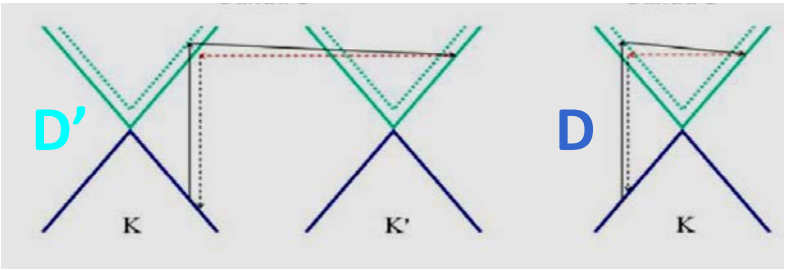
¡Hay que interpretar el espectro Raman del GO!

Espectro Raman de GO



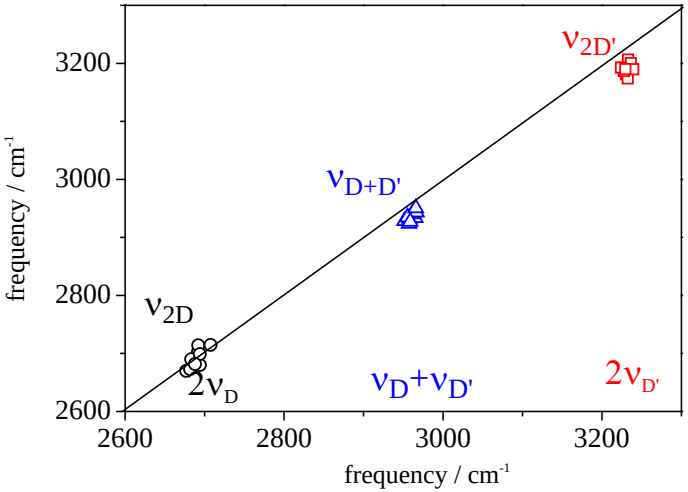
Grafeno: bandas G y 2D

Bandas D y D' (Doble Resonancia)
Acoplamiento fonón-electrón



Activadas por defectos

- D* → sp^3 (bordes del plano basal)
- D'' → Cristalinidad



Velázquez M.M. et. al. *J. Phys. Chem. C*, 119 , 10123, **2015**
Velázquez M.M. et al. *J. Phys. Chem. C* 121, 20489, **2017**

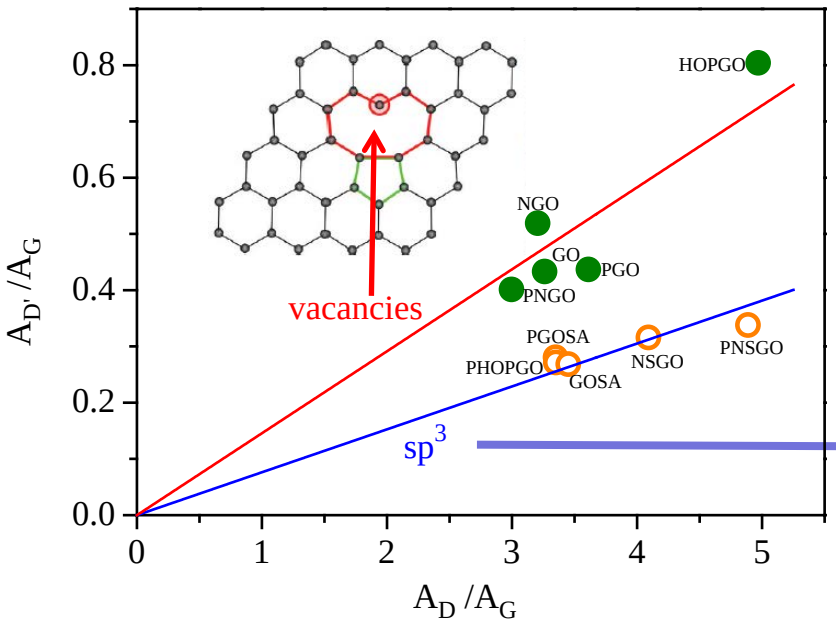
Espectro Raman de GO

Cálculos *ab initio* simulan el espectro Raman de grafeno con defectos

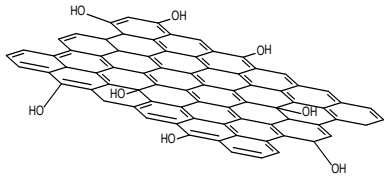
$I_D / I_G \leq 3.5$ → Grado de defectos bajo

Plaquetas grandes D > 400 nm

$A_{D'}/A_D = 0.143$



$A_{D'}/A_D = 0.077$

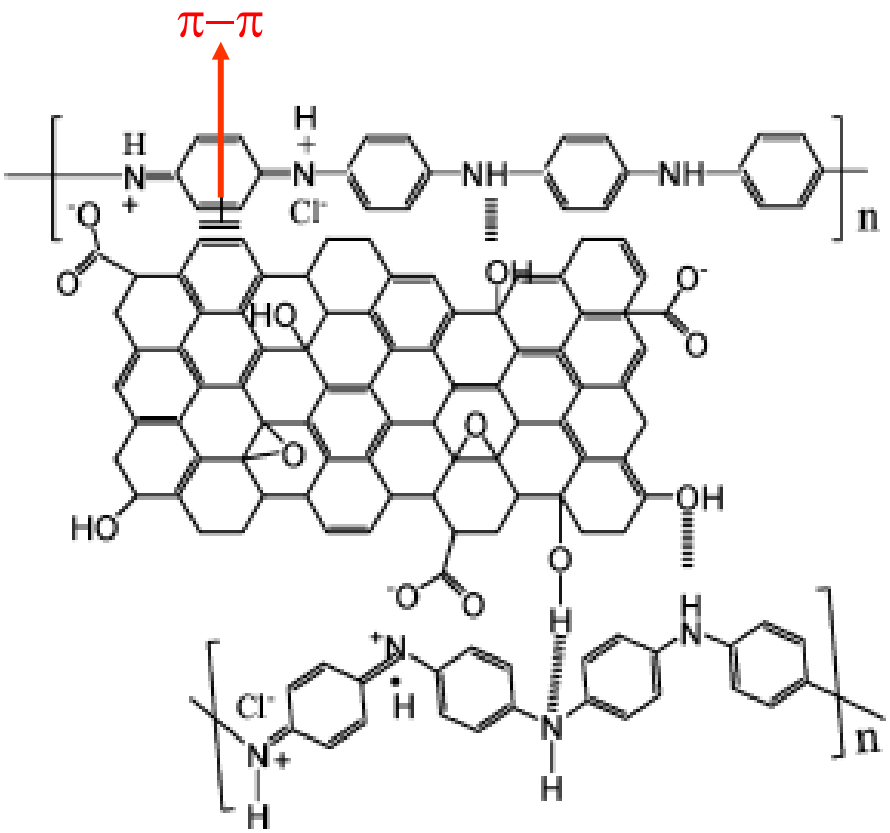


Plaquetas pequeñas D ~ 100 nm

Venezuela, P. et al. *Phys. Rev. B*, 84, 035433, **2011**.

Velázquez M.M.. *J. Phys. Chem. C*, 121, 20489, **2017**

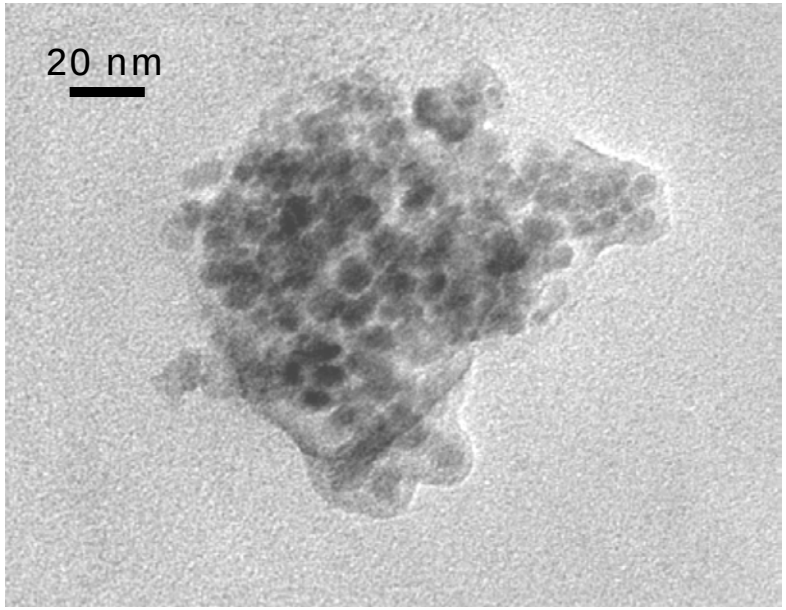
Híbridos GO + Polianilina (Retención de CO_2)



XPS
FT-IR
Raman
XRD

2 tipos de GO:
Oxidación de grafito (GOG)
Oxidación de nanofibras de carbono (GONF)

Híbridos GO + Fe_3O_4 (Retención de CO_2)



Area Superficial y Volumen de microporos

Adsorción N_2 (77 K)

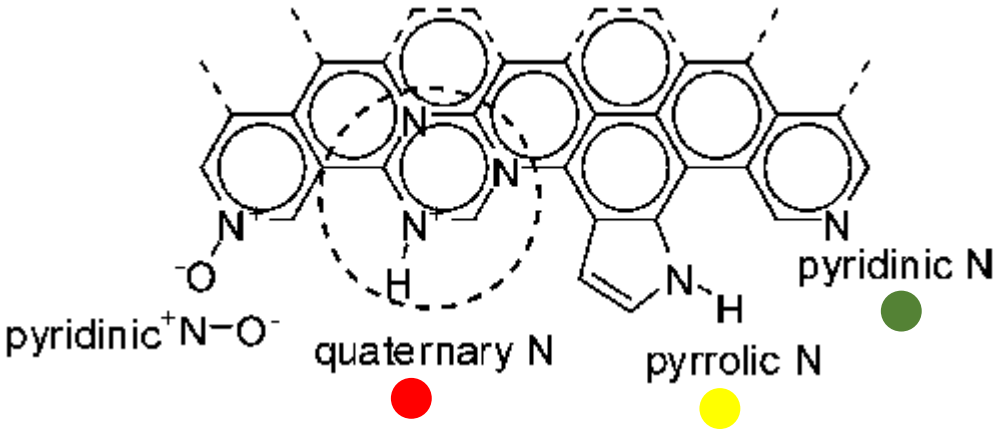
Modelo de BET

- Híbridos con polianilina **mayor** capacidad de retención de CO_2 y **menor** selectividad CO_2/N_2 que los híbridos con magnetita.
- Híbridos con óxido de grafeno procedente de nanofibras, **mayor selectividad**.

Grafeno Dopado con N

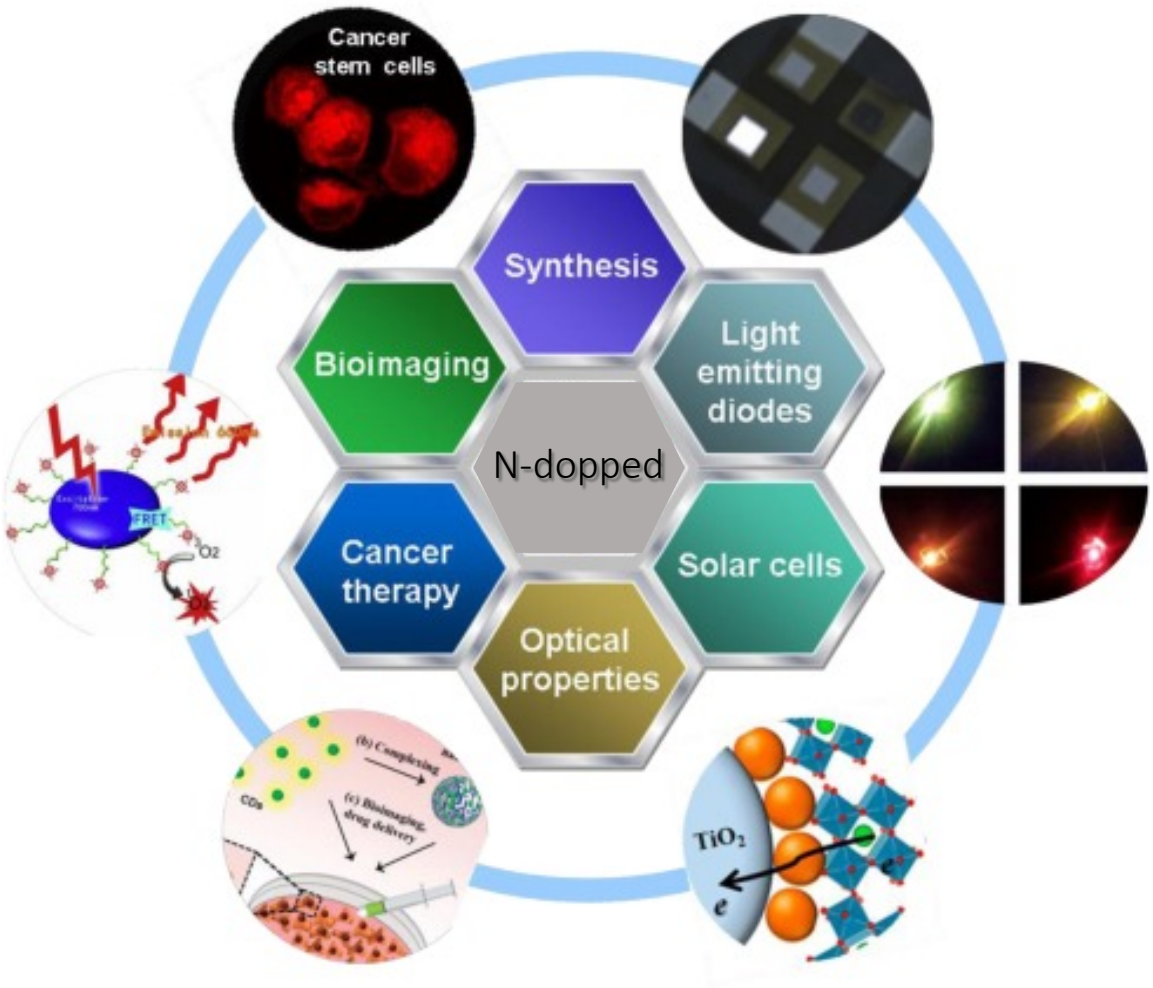
Obtención:

- Adsorción de gas, moléculas orgánicas nitrogenadas
- Introducción de los Heteroátomos en la red (CVD, arc-discharge)

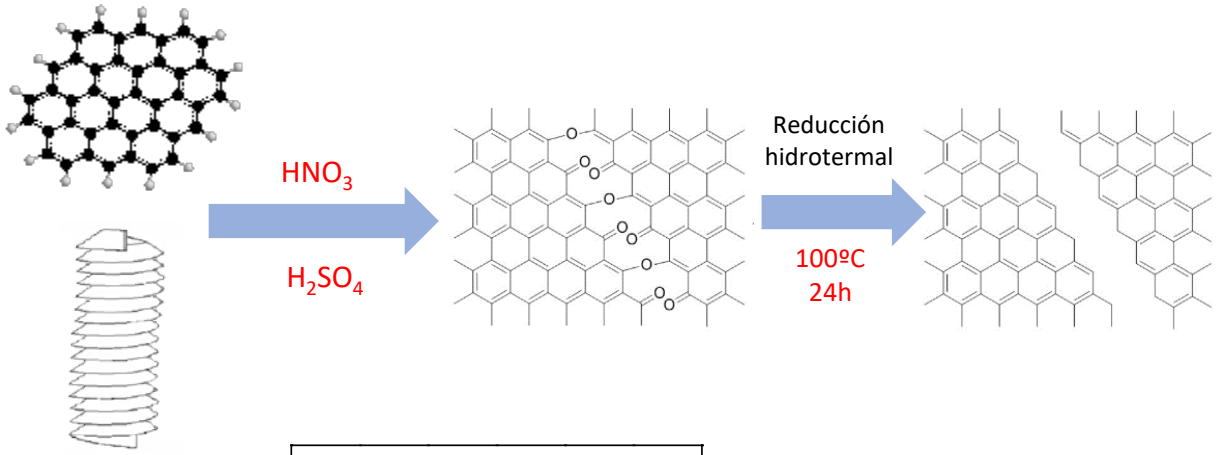


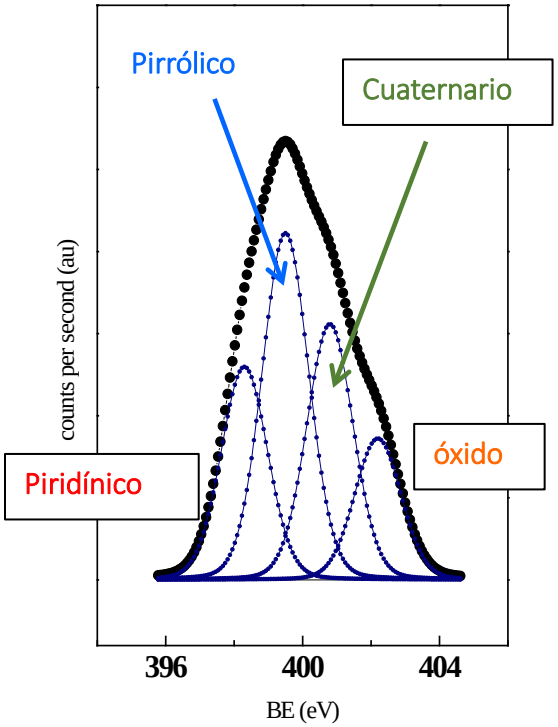
- Regiones activadas usadas como catalizadores, para anclar NP, etc.
- Band gap aumenta

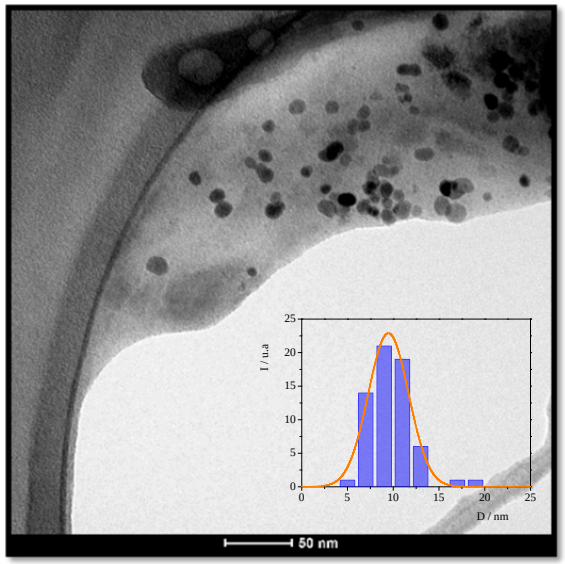
Grafeno Dopado con N: aplicaciones



Grafeno Dopado con N: Puntos de grafeno, Grafeno Dots







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¿Son los derivados de grafeno el futuro de este material?

Lunes, 12 de marzo, 13:00 h.
Aula III (edificio Trilingüe)

Mercedes Velázquez

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