

Desarrollo de tecnologías para celdas solares fotovoltaicas basadas en nanomateriales

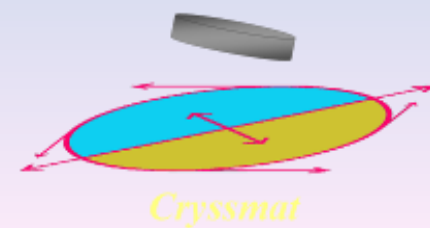
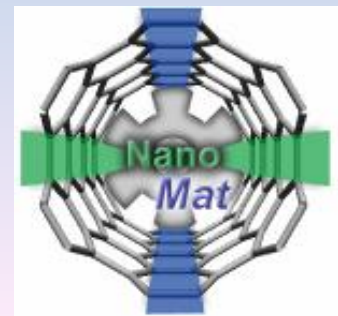
Responsable: Alvaro Mombrú

Cryssmat-Lab. DETEMA.

Facultad de Química

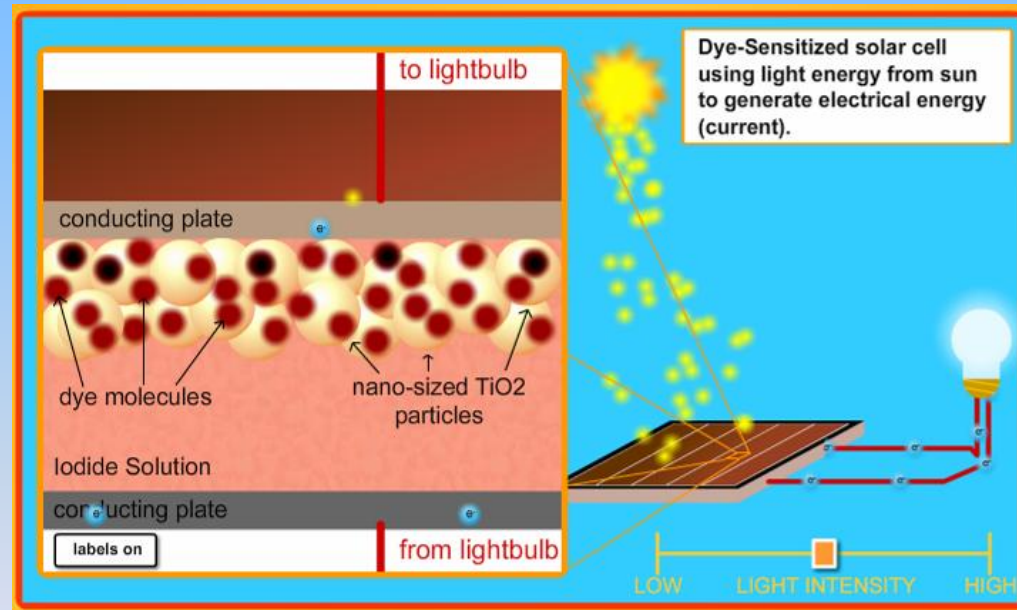
Centro NanoMat PTP-Pando,

Facultad de Química



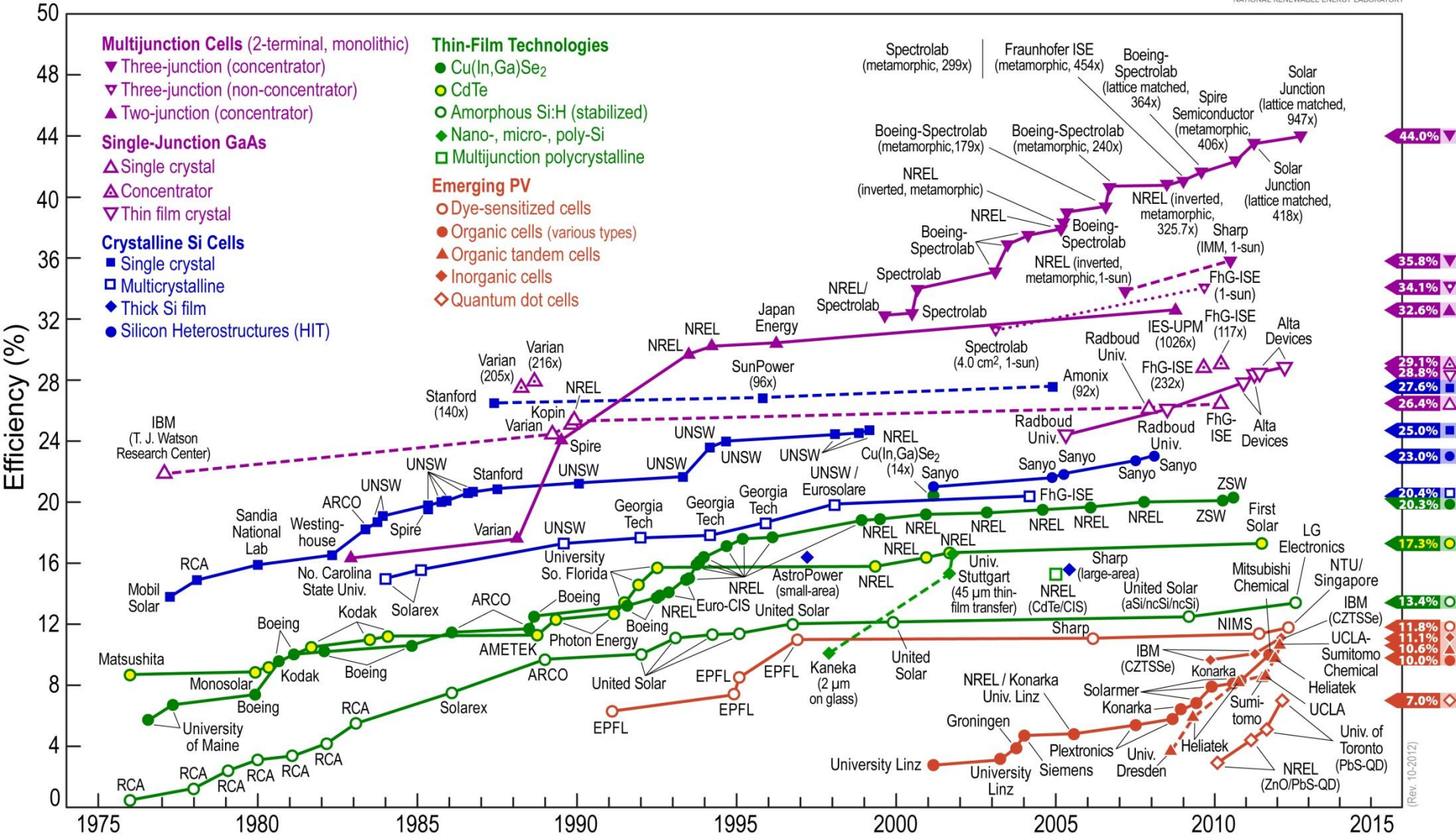
Aprovechamiento de la Energía Solar

- Sol
- Limpia y renovable
- Convertible

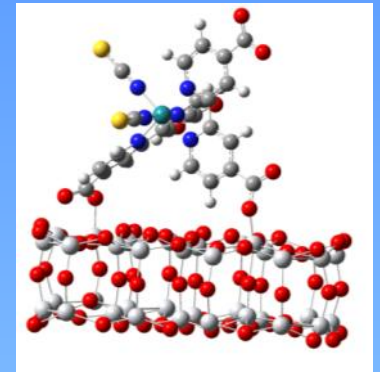


Panel solar -
fotovoltaico

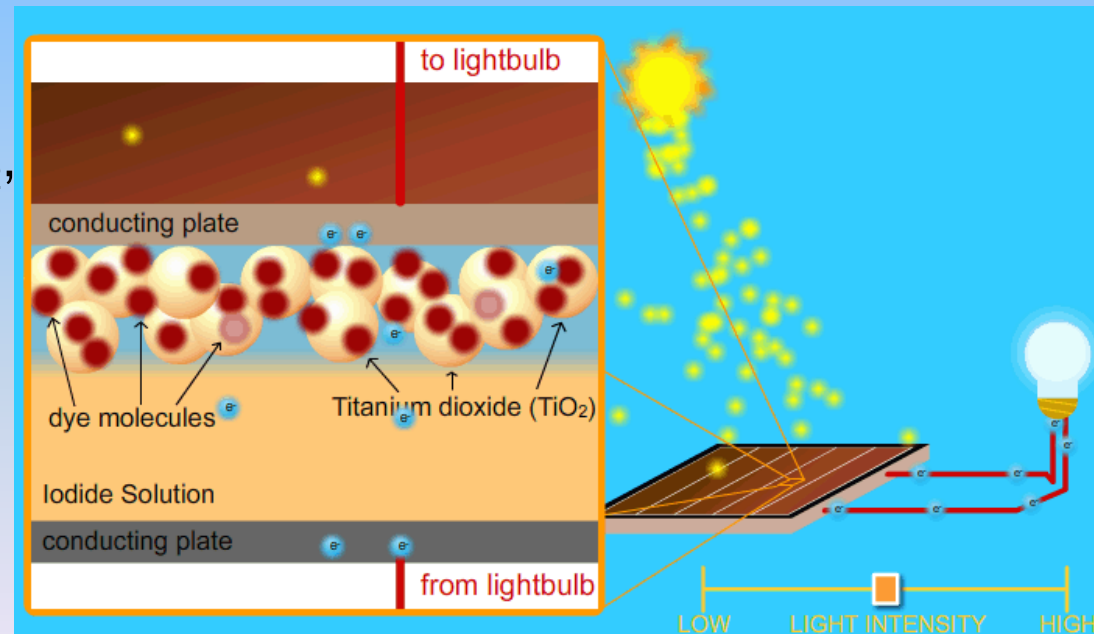
Best Research-Cell Efficiencies



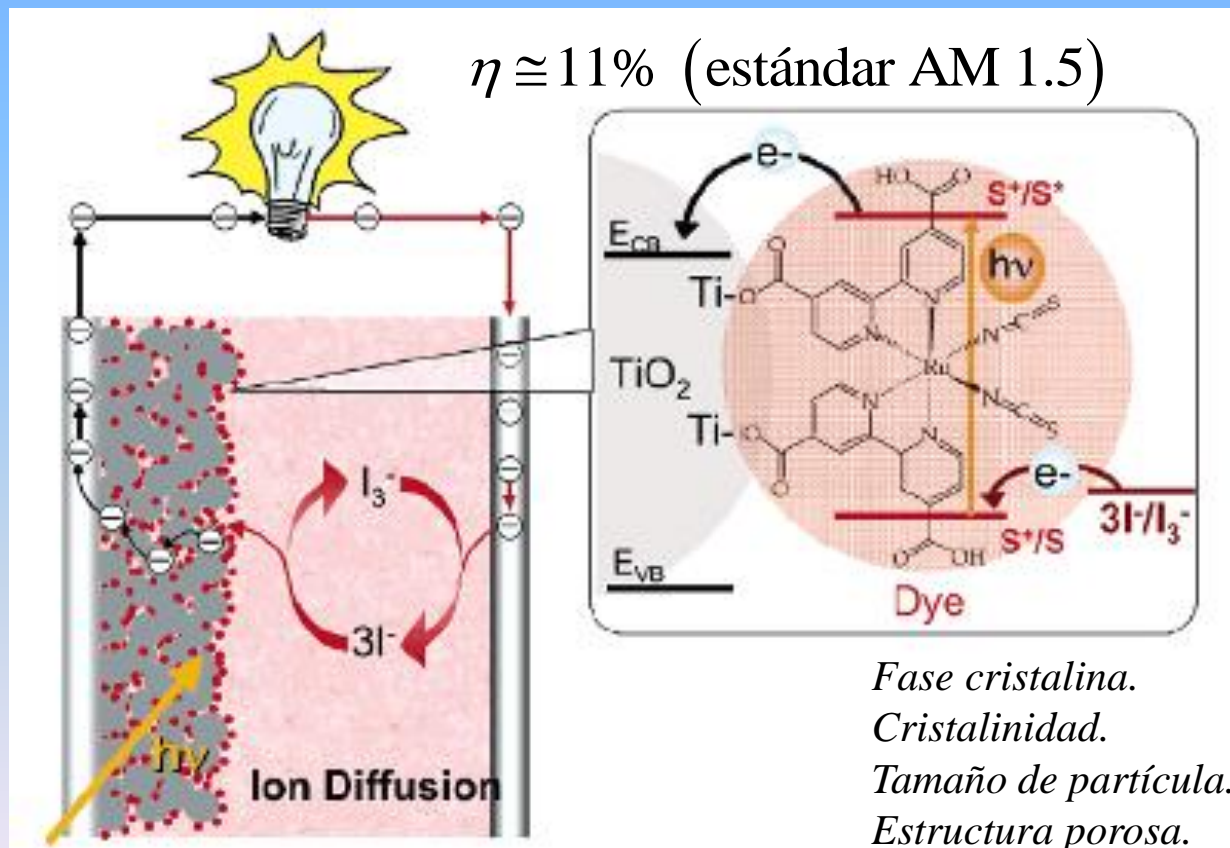
Celdas Solares DSSC



- Funcionamiento equivalente a las de Si
- Los electrones se arrancan del colorante y se inyectan en TiO_2 , para transportarlo fuera de la celda
- Los “huecos” permanecen en la tinta
- La separación hueco-electrón genera un voltaje y corriente



Celdas solares de sensibilización espectral (Celdas solares sensibilizadas con colorantes, DSSC)



Fase cristalina.
Cristalinidad.
Tamaño de partícula.
Estructura porosa.

- Foto-electrodo
 - Conductor
 - Semiconductor
 - Colorante
- Contraelectrodo
 - Conductor
 - Catalizador
- Electrolito

TiO_2

- Bajo costo
- Ampliamente disponible
- No tóxico
- Biocompatible

• Grätzel M., *Inorg. Chem.* **2005**, *44*, 6841

• Faccio, R; Fernández-Werner, L.; Pardo, H.; W. Mombrú, A. *Recent Patents on Nanotechnology* **2011**, *5*(1), 46-61.

Síntesis

Método hidrotermal
bajo presión endógena



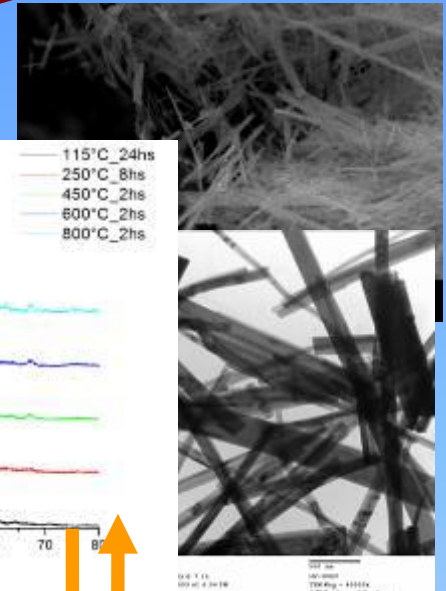
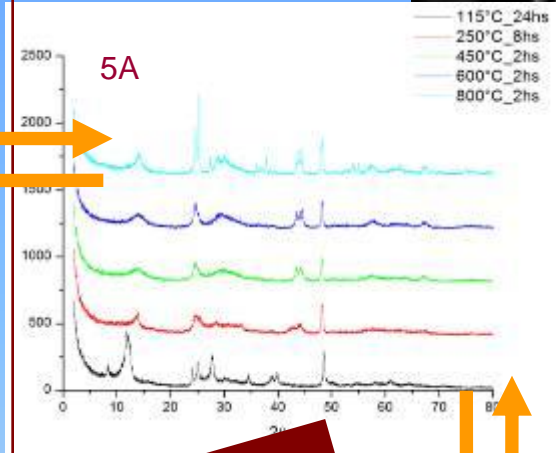
NaOH(ac) 10M

$120^{\circ}\text{C} < T_r < 150^{\circ}\text{C}$

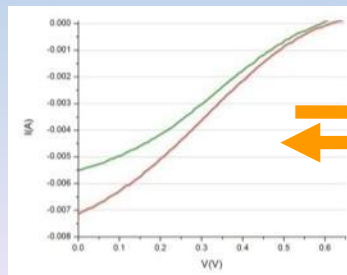
$24\text{h} < t_r < 68\text{h}$

(A, R, o A/R 50% p/p)

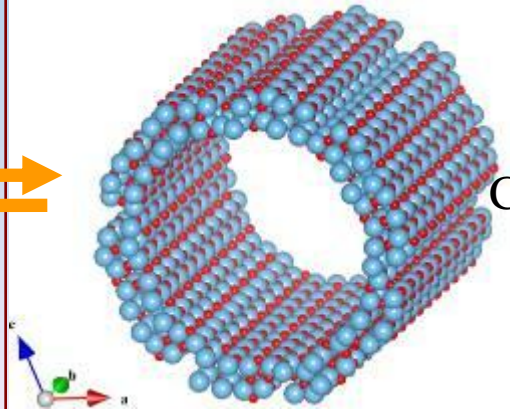
Caracterización



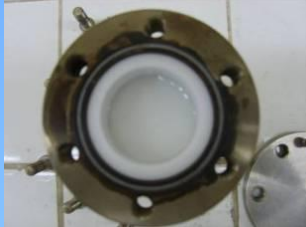
Prototipos

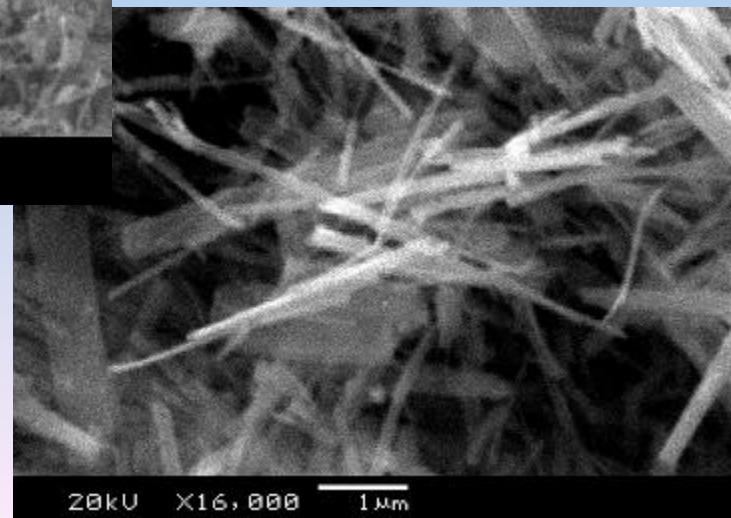
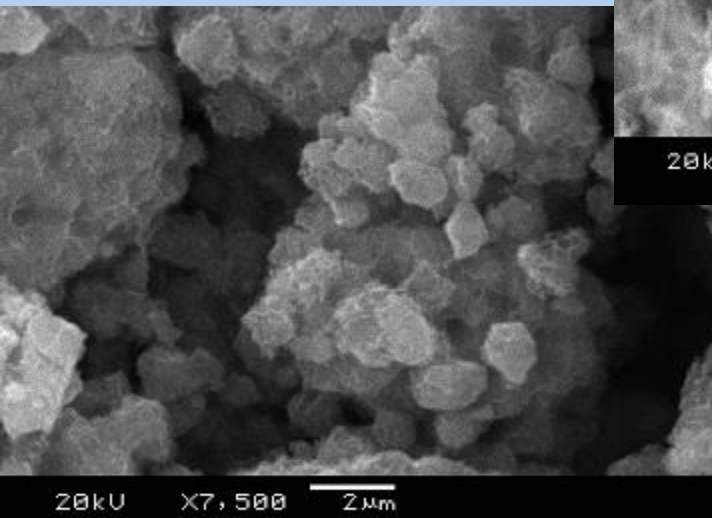
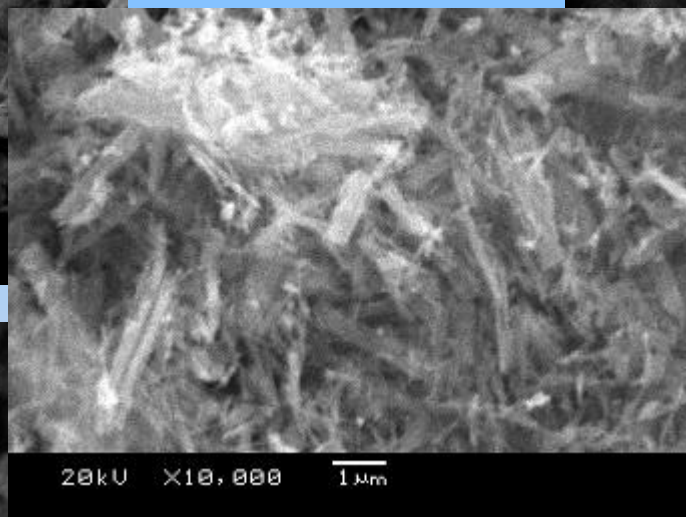
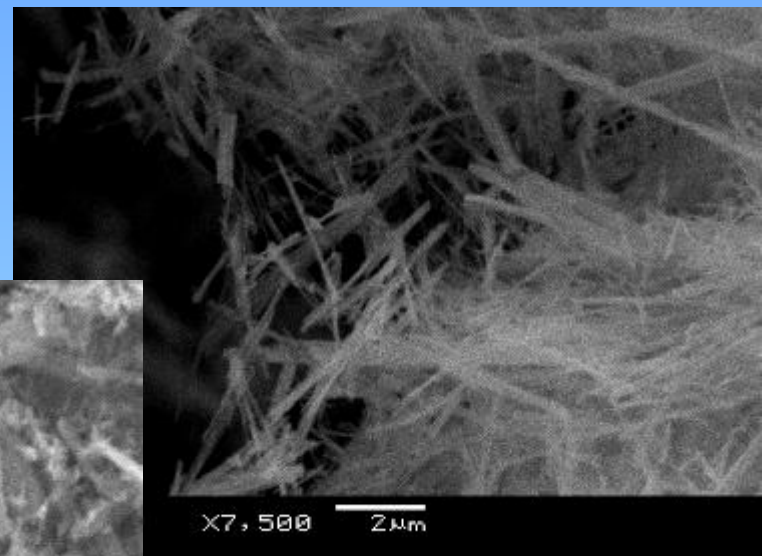
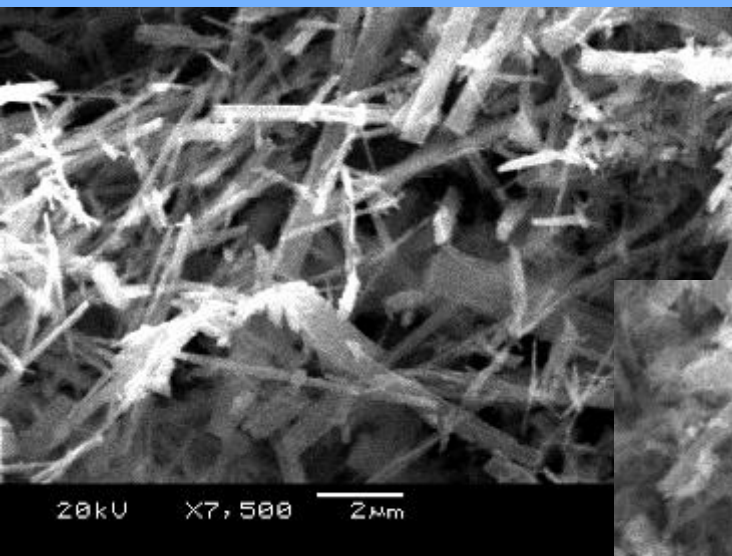


Modelado

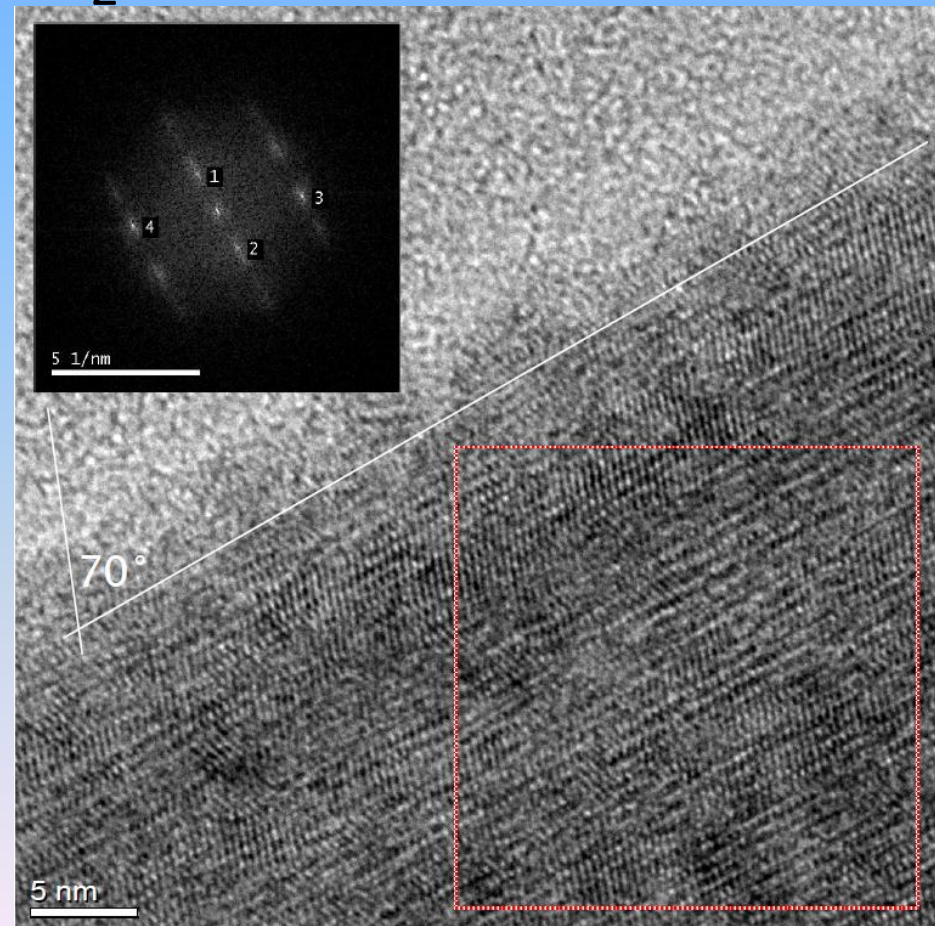
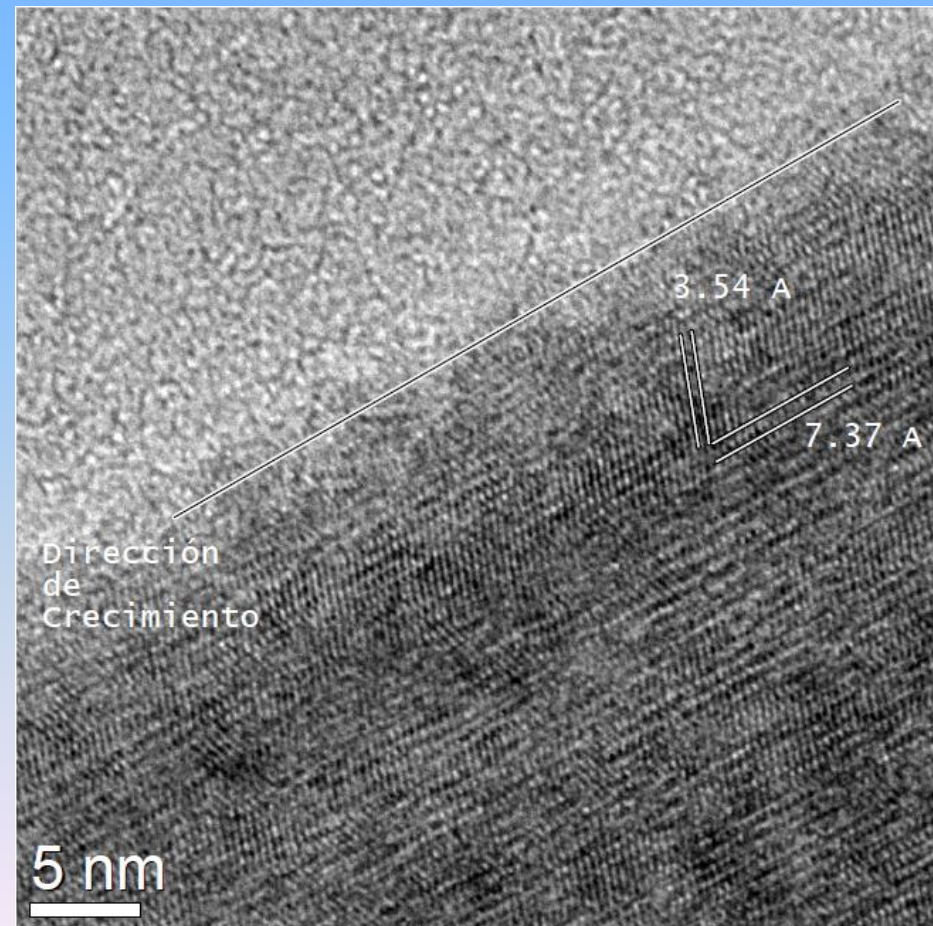


Cálculos teóricos
por *primeros principios*

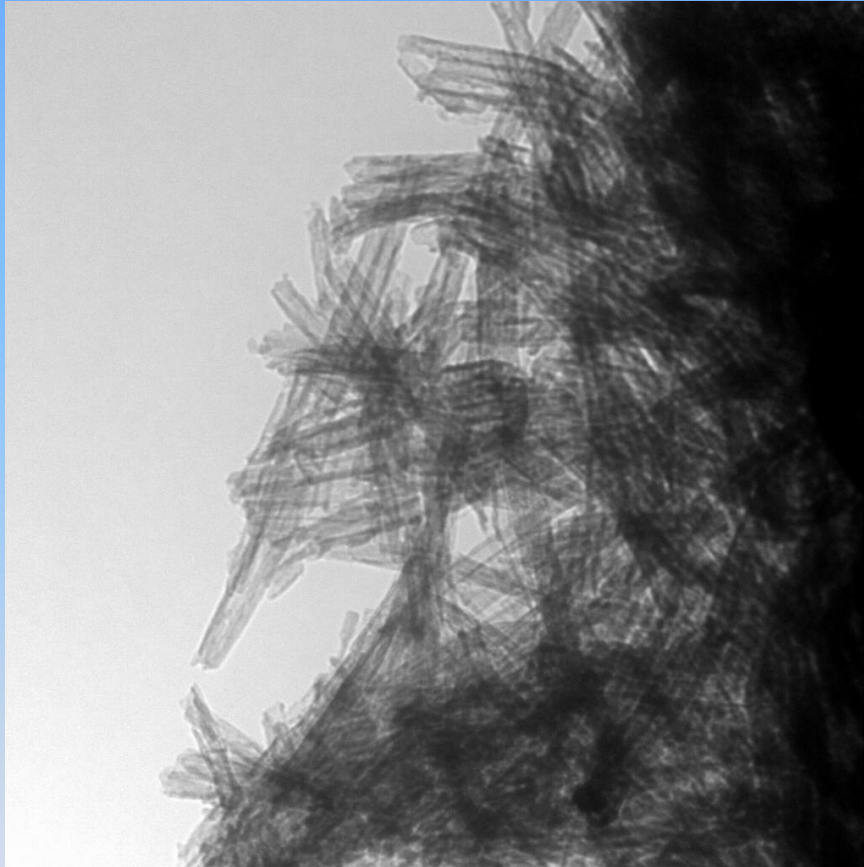




- HRTEM: nanorods de TiO_2



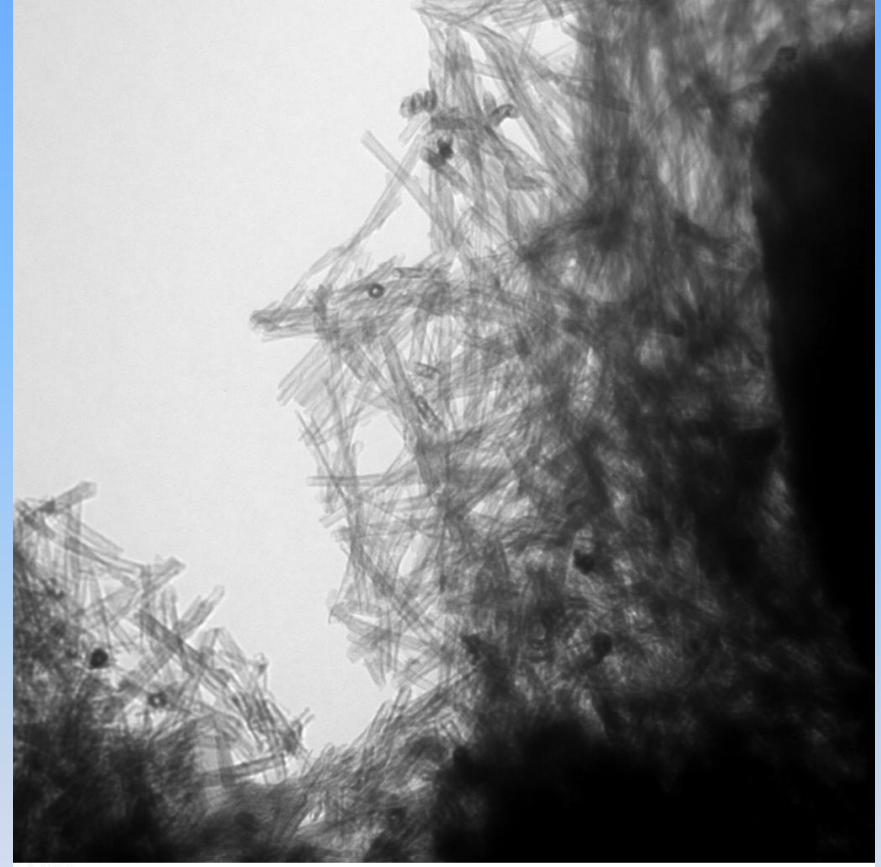
TEM: Nanotubos de TiO_2



15 002

Print Mag = 13979x @ 6.99999969005585 mm
Acquired Oct 2 2012 at 11:41 AM

100 nm
HV=100kV
TEM Mag = 250000x
AMT Preferred Customer

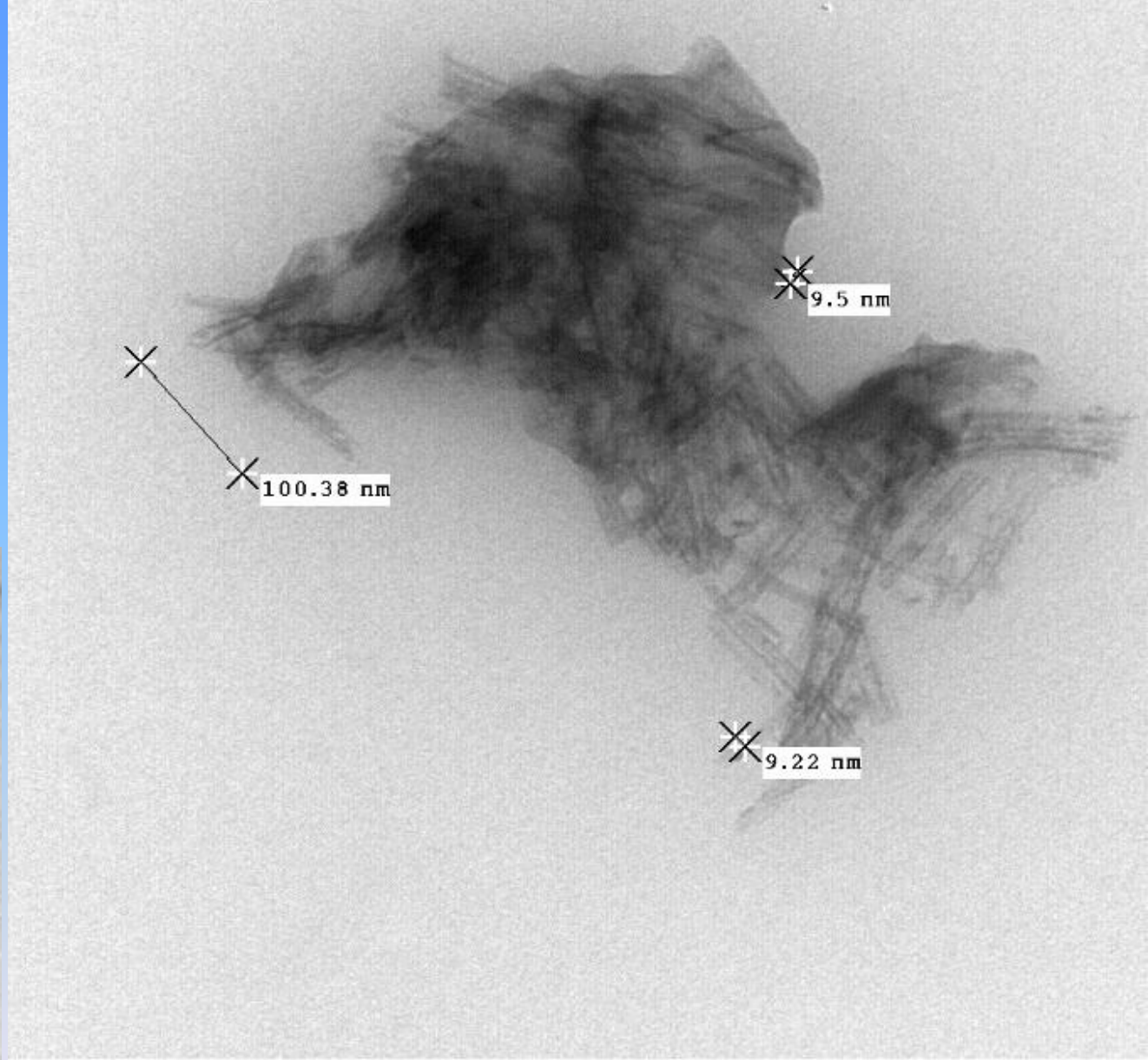
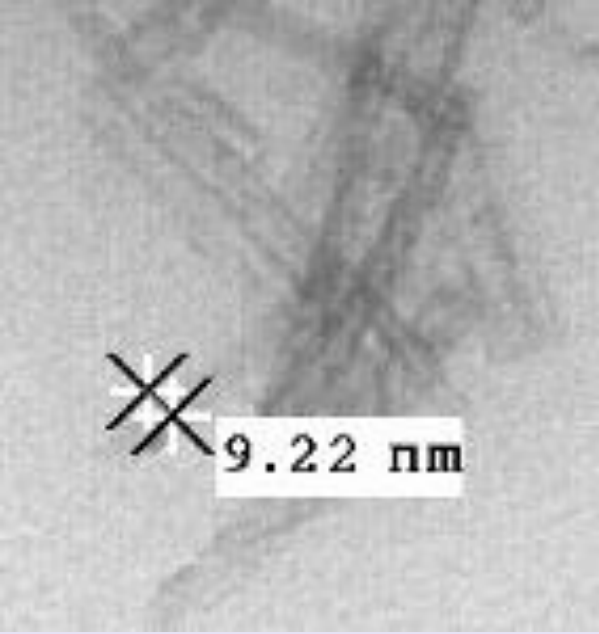


15 005

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Acquired Oct 2 2012 at 11:46 AM

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AMT Preferred Customer

- TEM:
-Nanotubos



BI TiO2 001

Acquired Mar 30 2012 at 9:15 AM

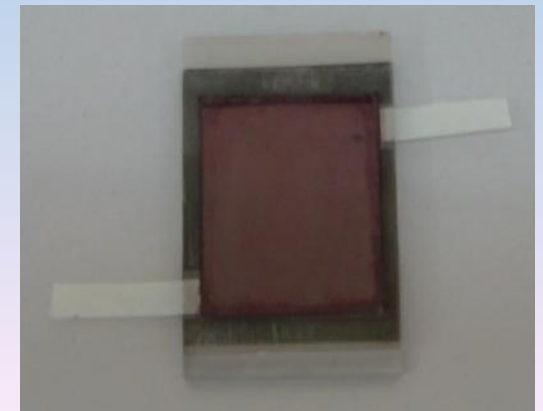
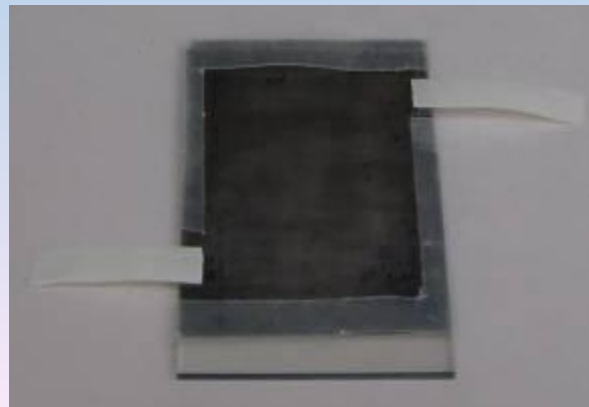
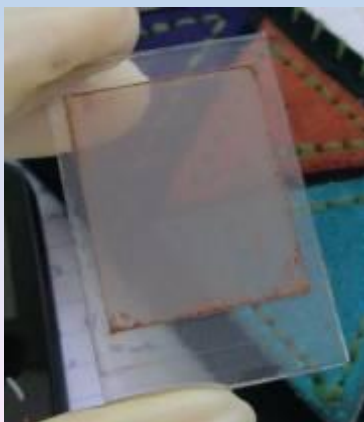
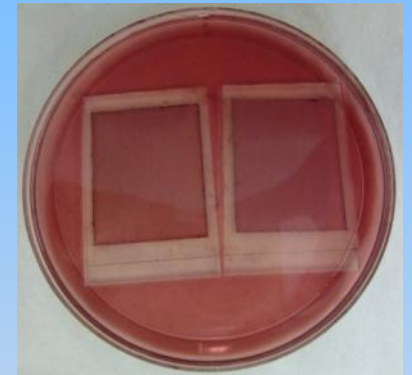
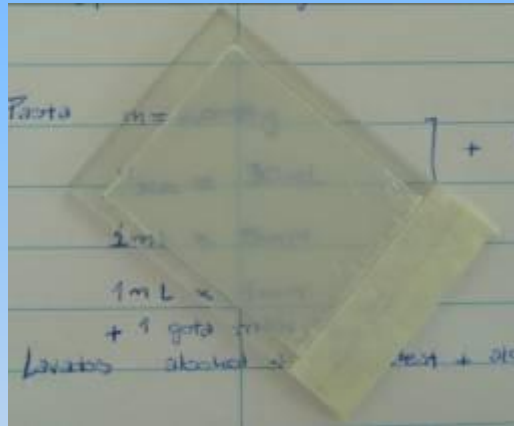
100 nm

HV=100kV

TEM Mag = 150000x

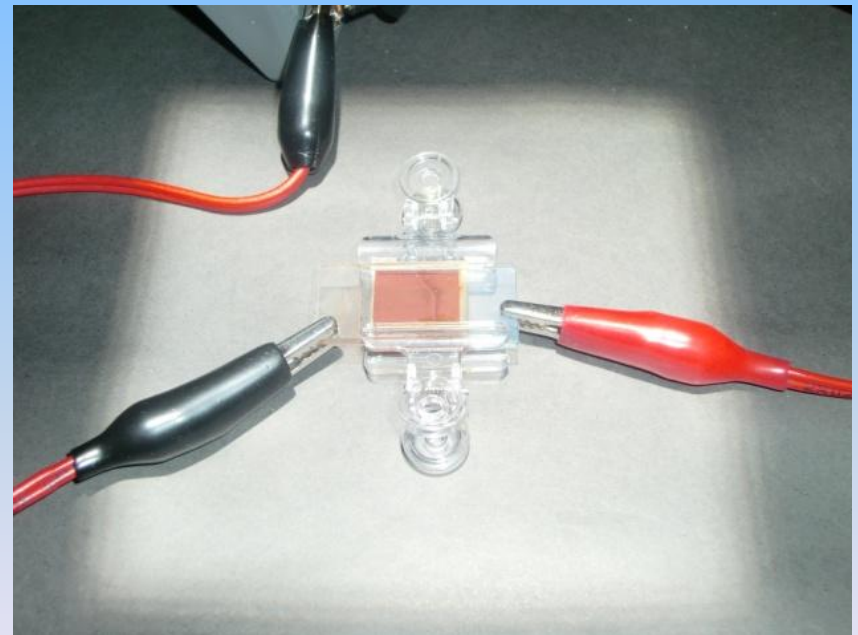
AMT Preferred Customer

- Ensamblado de Dispositivos

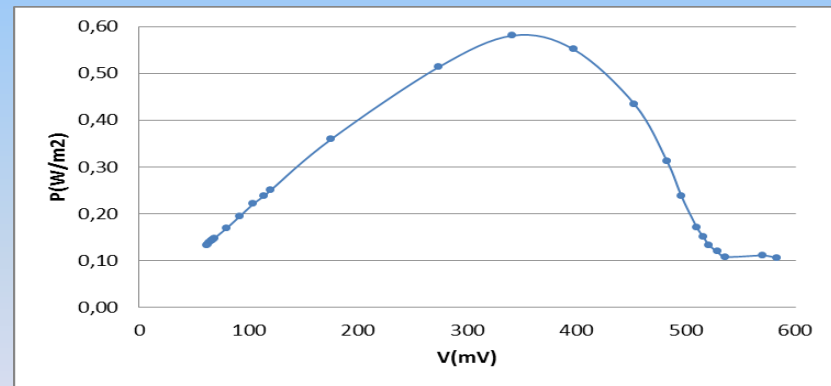
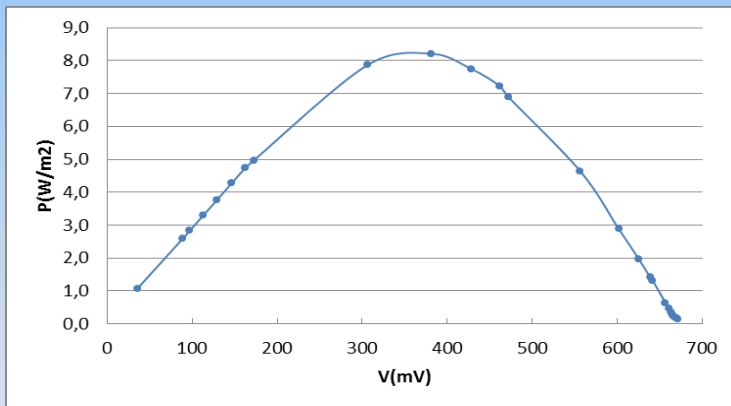
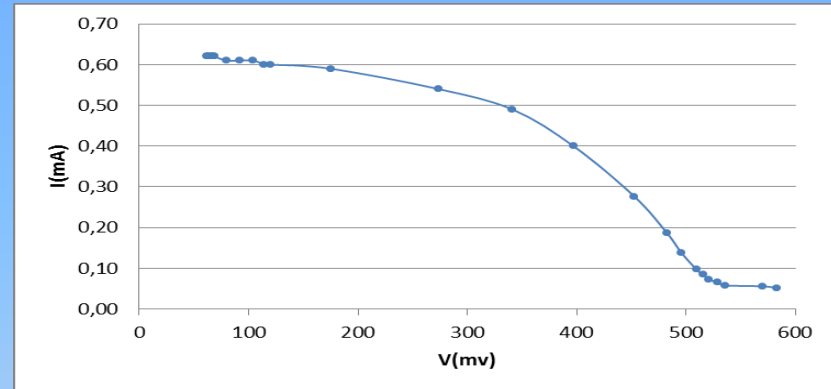
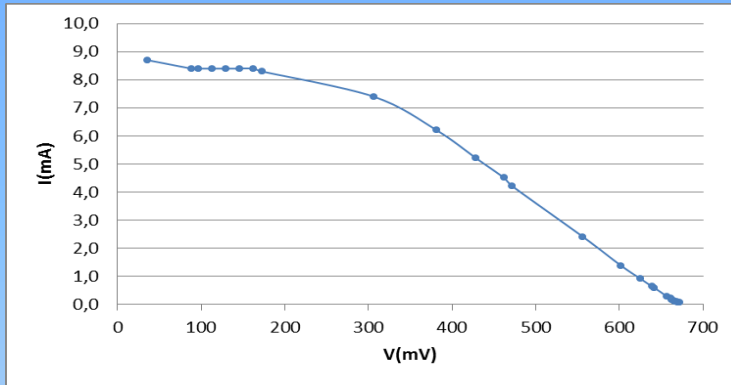


Simulador Solar:

- *Solar Cell Testing 1000W Light Source – Model LS1000* de Solar Light el cual provee $1000\text{W}/\text{m}^2$ AM 1,5 en el plano de trabajo



Caracterización Eléctrica



Prototipo	I_{sc} (mA)	J_{sc} (mA/cm ²)	V_{oc} (mV)	FF (%)	η (%)
1	9.0	3.1	680	39	0.82
2	0.62	0.22	590	46	0.06

Preparación de óxidos precursores para CIGS

- Los precursores óxido de cobre e indio han sido sintetizados por el método de complejación-combustión de Pechini usando ácido cítrico y etilenglicol.
- Las cantidades requeridas de $\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$ e $\text{In}(\text{NO}_3)_3 \cdot 4\text{H}_2\text{O}$ son disueltas en agua desionizada a $T=50^\circ\text{C}$ bajo agitación y se agrega ácido cítrico (AC) y etilenglicol (EG) en la siguiente relación molar $M:\text{AC}:\text{EG} = 1:2:2$.
- La solución obtenida es calentada a $90\text{-}100^\circ\text{C}$ durante 5 horas hasta la formación del gel, luego es secado a 150°C durante 4 horas (CIS_1) y posteriormente calcinado a 500°C durante 8 horas para obtener los óxidos precursores (CIS_2).

Preparación de tintas para películas delgadas

- Se ensaya la preparación de la pasta para realizar el depósito de la película fina del precursor por el método de spin-coating.
- La pasta está compuesta por butil-carbitol (BC-solvente), etilcelulosa (EG-sellante) y polietilenglicol (PEG-dispersante) | en la relación en peso CIS_2:PEG:EC:BC que se detallan a continuación:

	CIO (mg)	PEG (mg)	EC (mg)	BC (mL)	N (80seg.)	Speed (rpm)
1:1.5:2:60	30,8	46,2	61,6	1,5	3 <u>coatings</u>	1500-2500

- El depósito es calentado a 600°C en mufla durante 4 horas para eliminar los componentes de la pasta y obtener así la película de los óxidos precursores (CIS_2) sobre el sustrato vidrio:ITO (óxido de indio y estaño).
- La sulfuración se realiza a 450°C en flujo de Ar 99.9% en presencia de exceso de azufre en una zona de T= 300°C durante 1 hora (CIS_3).

Buscando alternativas

Buscando nichos

**Leijtens et al, Nature Comm. DOI:
10.1038/ncomms3885**

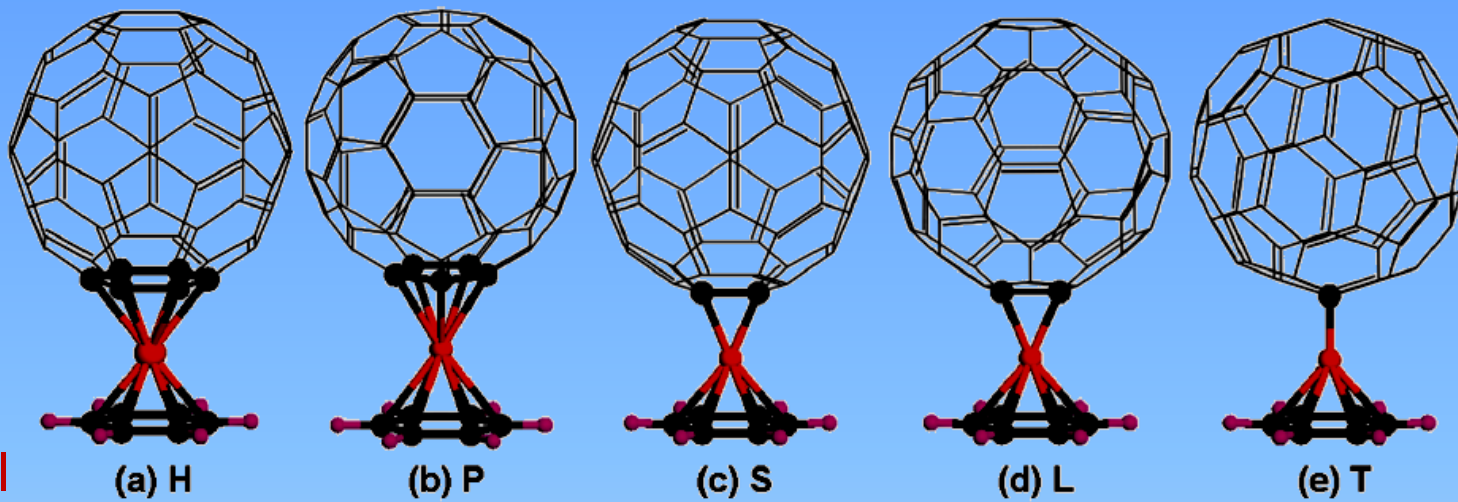
Celdas basadas en Perovskitas

**A la búsqueda de captar fotones en
el infrarrojo**

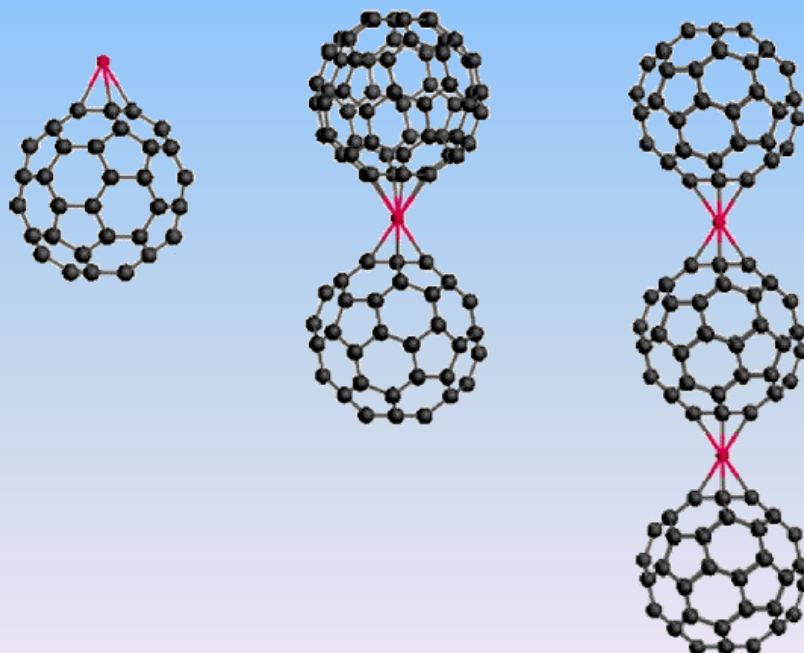
**Se usa una aproximación a través
de un nanomaterial híbrido**

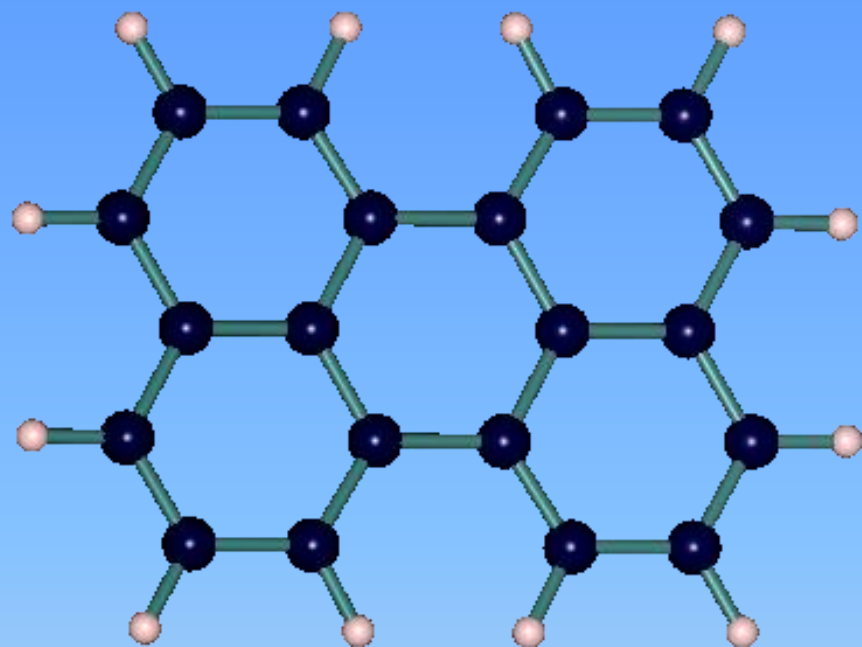
Acceptor – M – Donor

Zhu et al



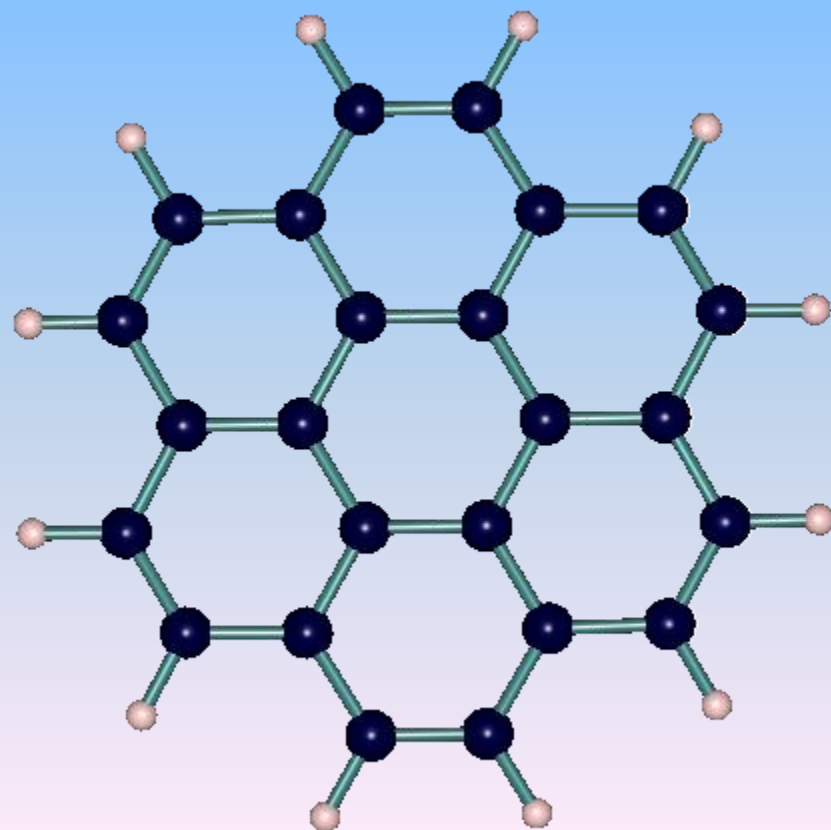
Zhang et al

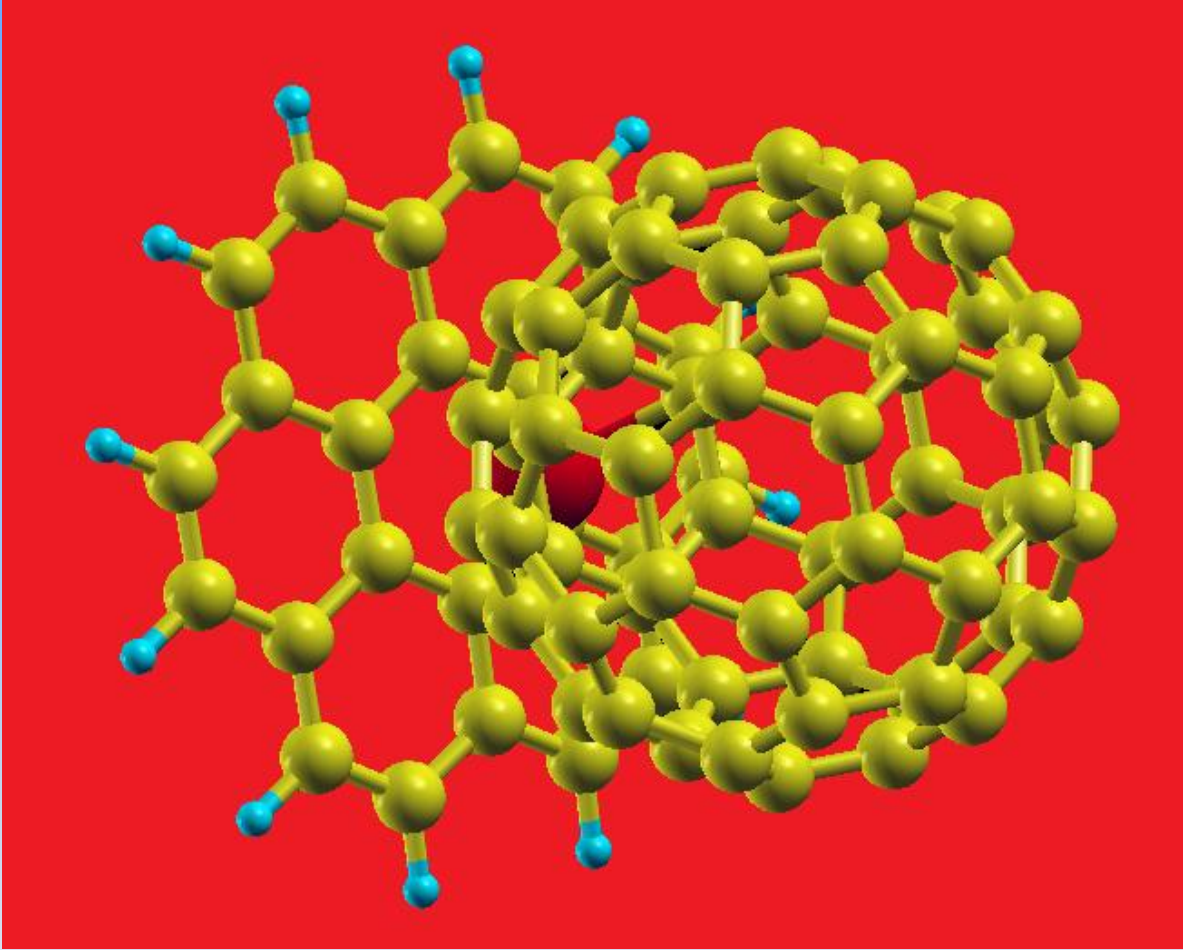




Coronene D_{6h}

Perylene D_{2h}

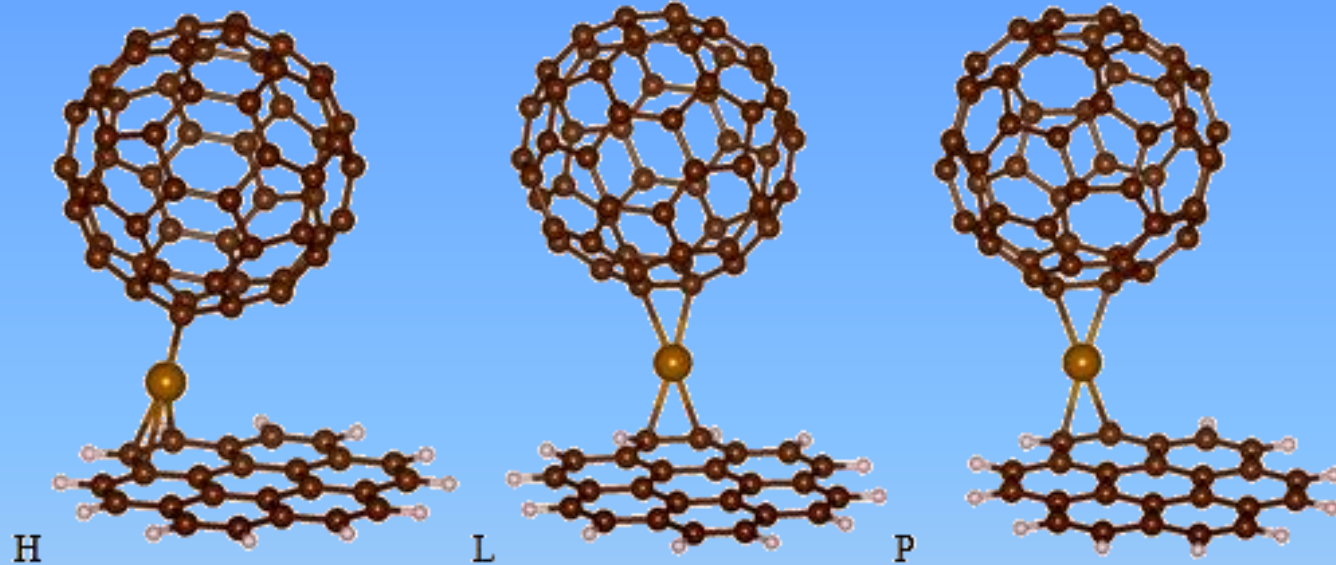




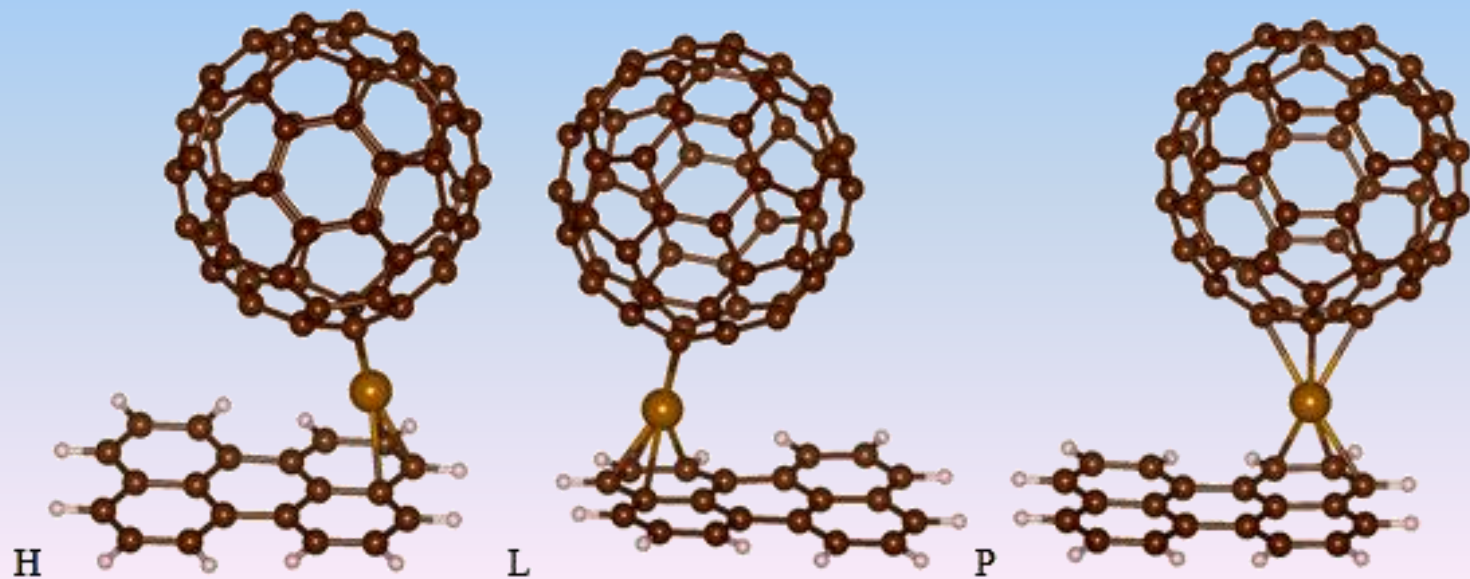
Coronene

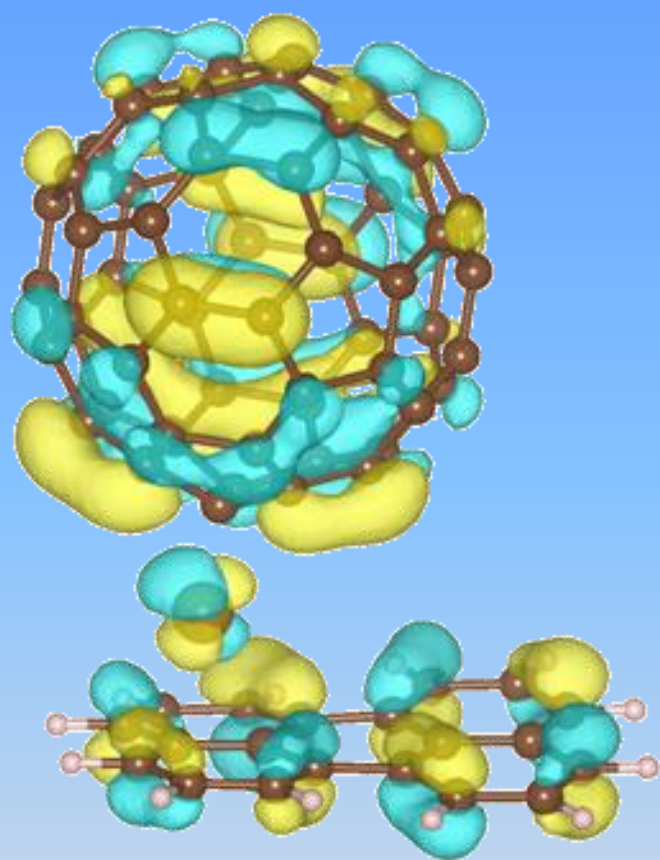
Coronene Fe at Hollow position

Faccio et al, 2013

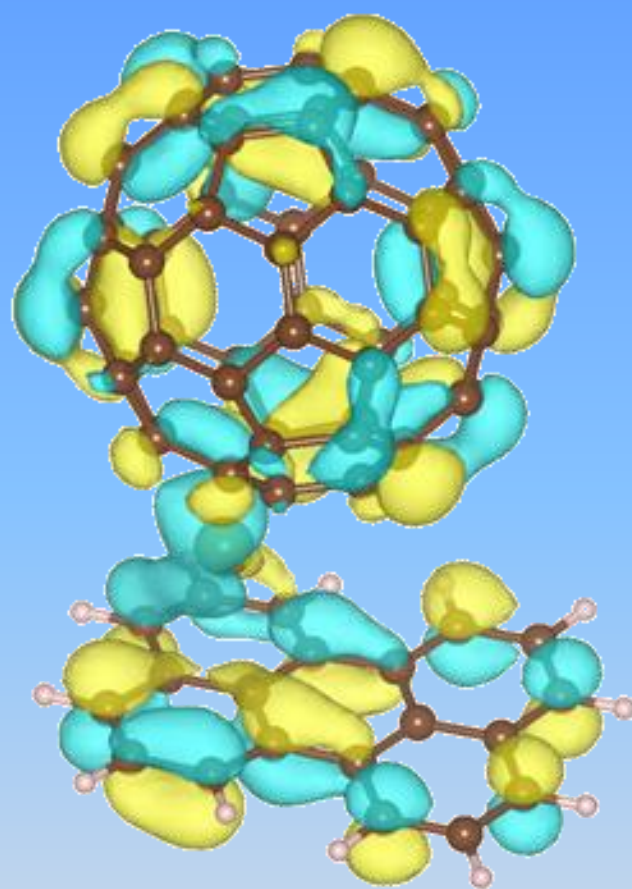


Perylene Fe at Hollow position





HOMOa

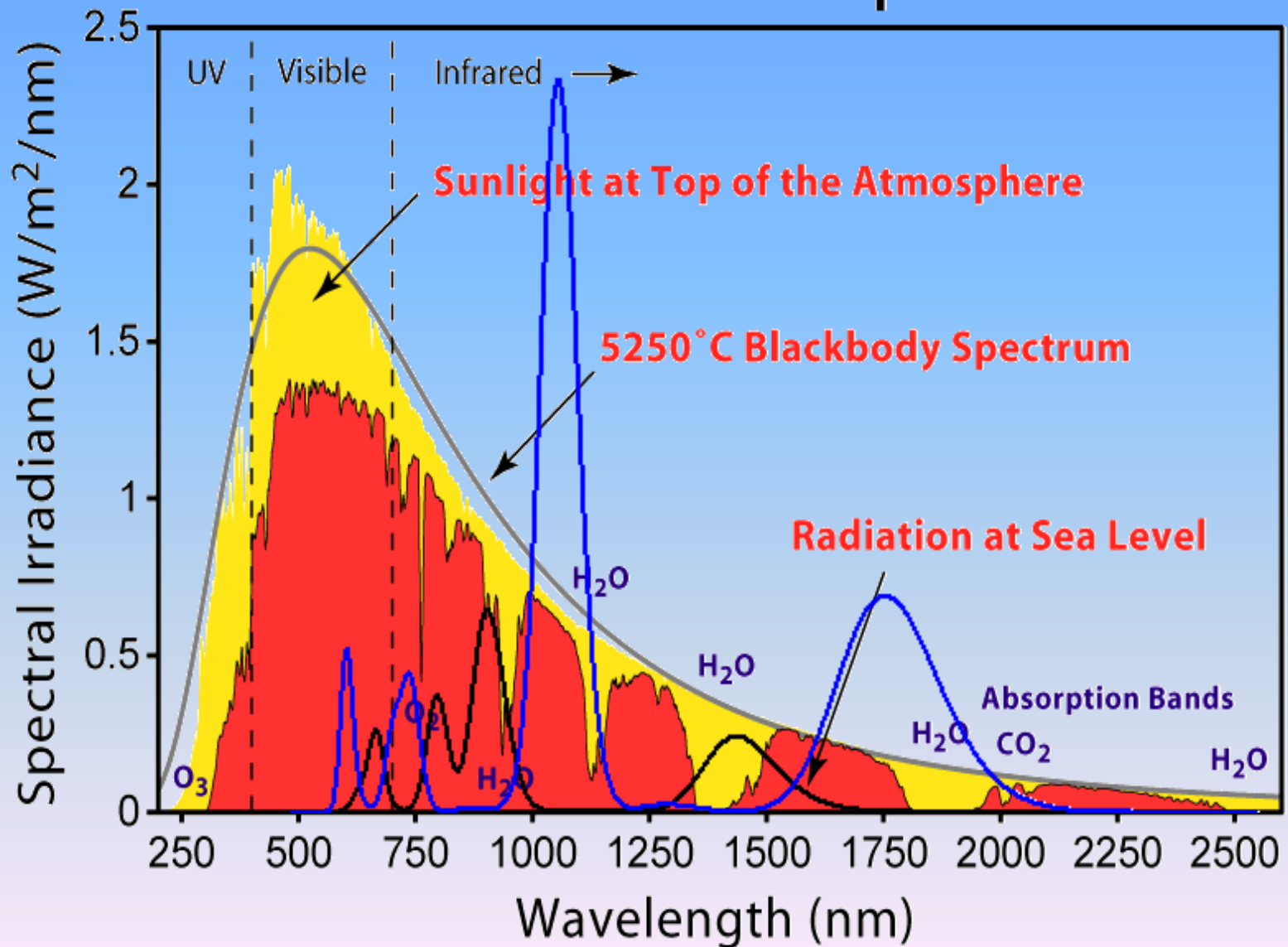


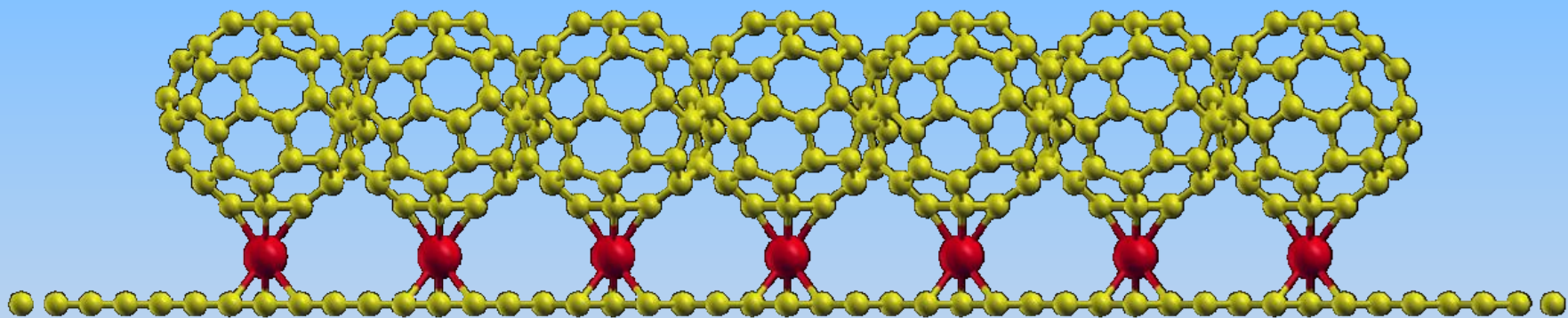
LUMOa

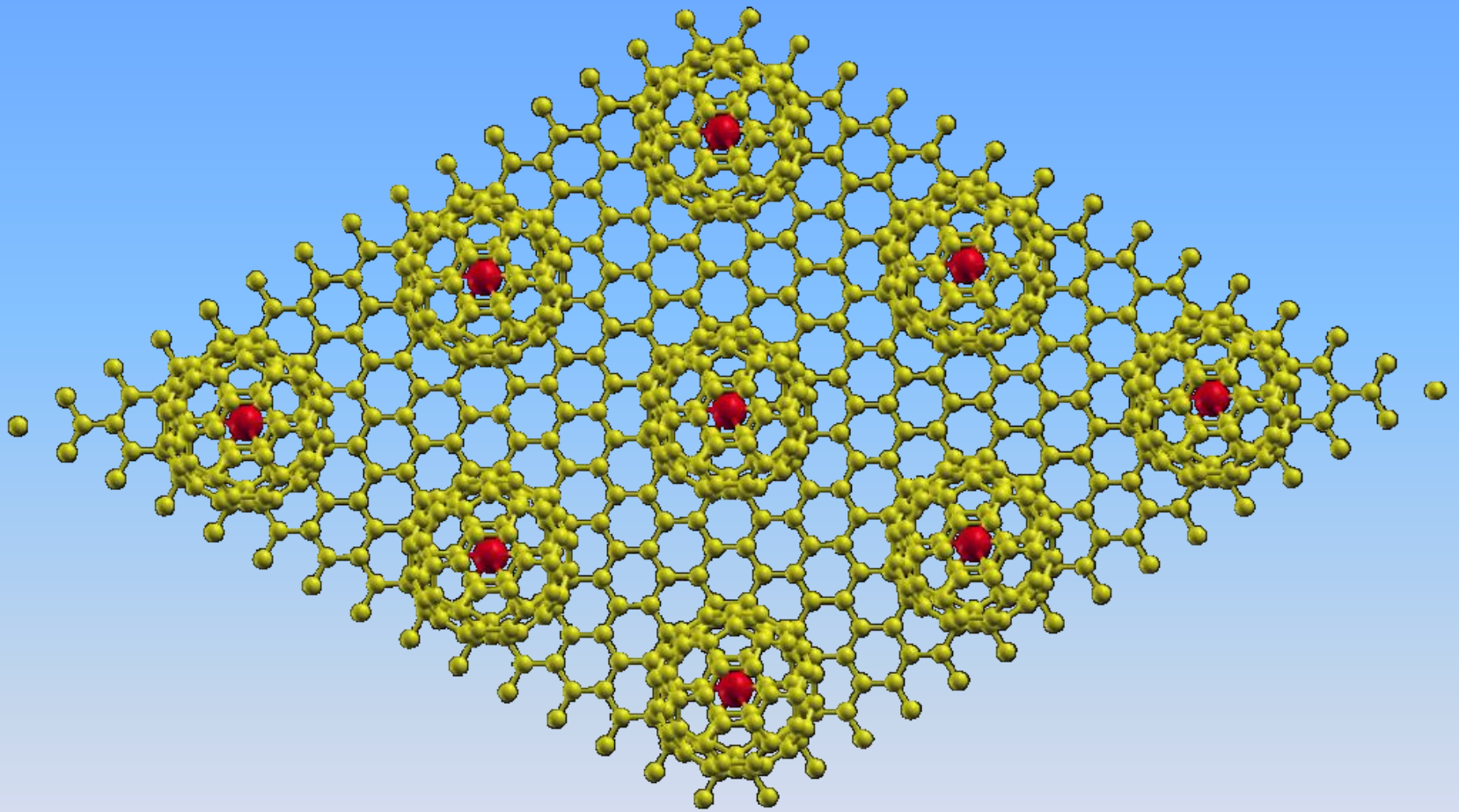
Perylene

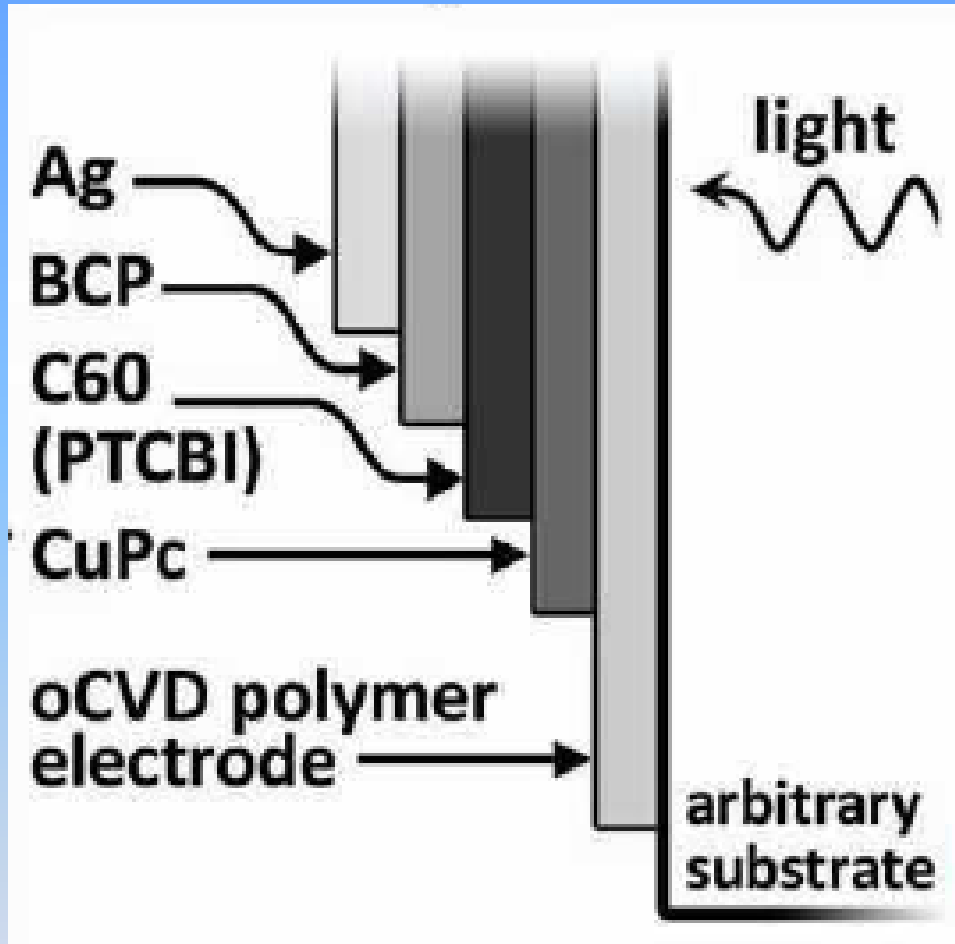
L

Solar Radiation Spectrum









Barr et al, Adv. Mater. 2011, 23, 3500-3505

Geometrías de Haz de Rayos X

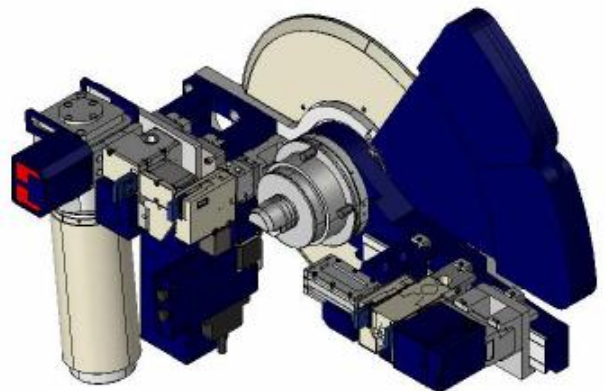
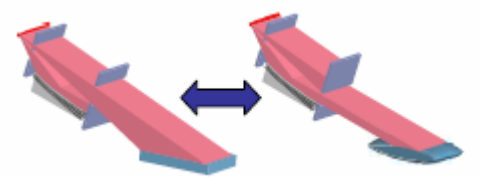
- Geometría Para focalizante Bragg-Brentano
- Geometría Haz paralelo, Cross-Beam-Optics CBO



Multi Purpose Attachment:

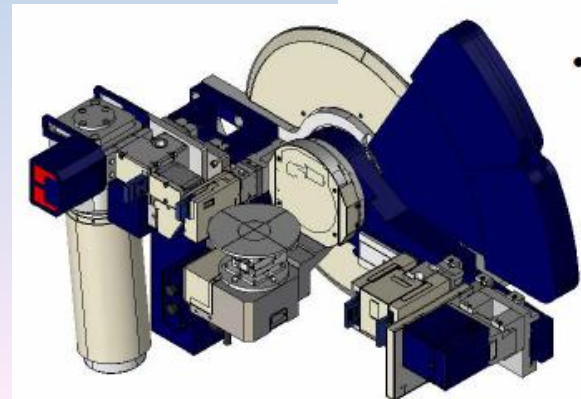
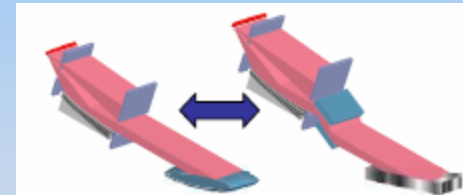
- Parallel Beam

- Superficies rugosas y curvas
- Textura
- Stress residual
- Estructuras nanoporosas, distribución de tamaño



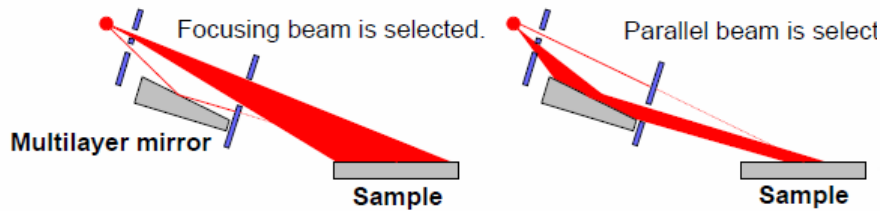
- Thin Films

- Espesor, densidad y rugosidad de films
- Caracterización epitaxial
- GIXRD

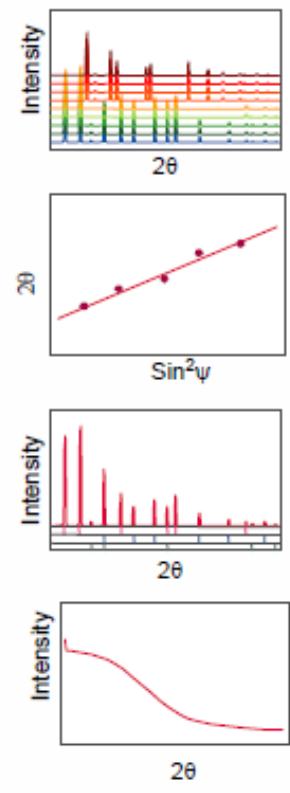
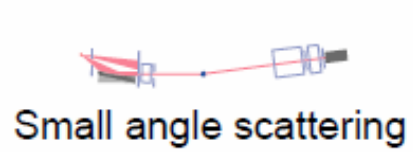
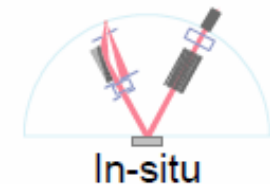
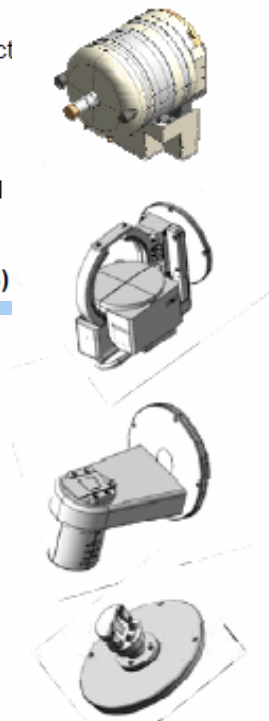
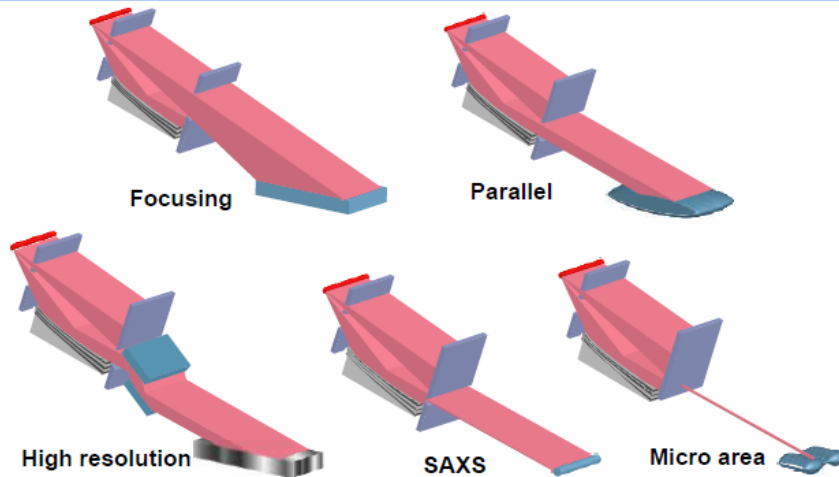


Variedad de Configuraciones

X-ray source

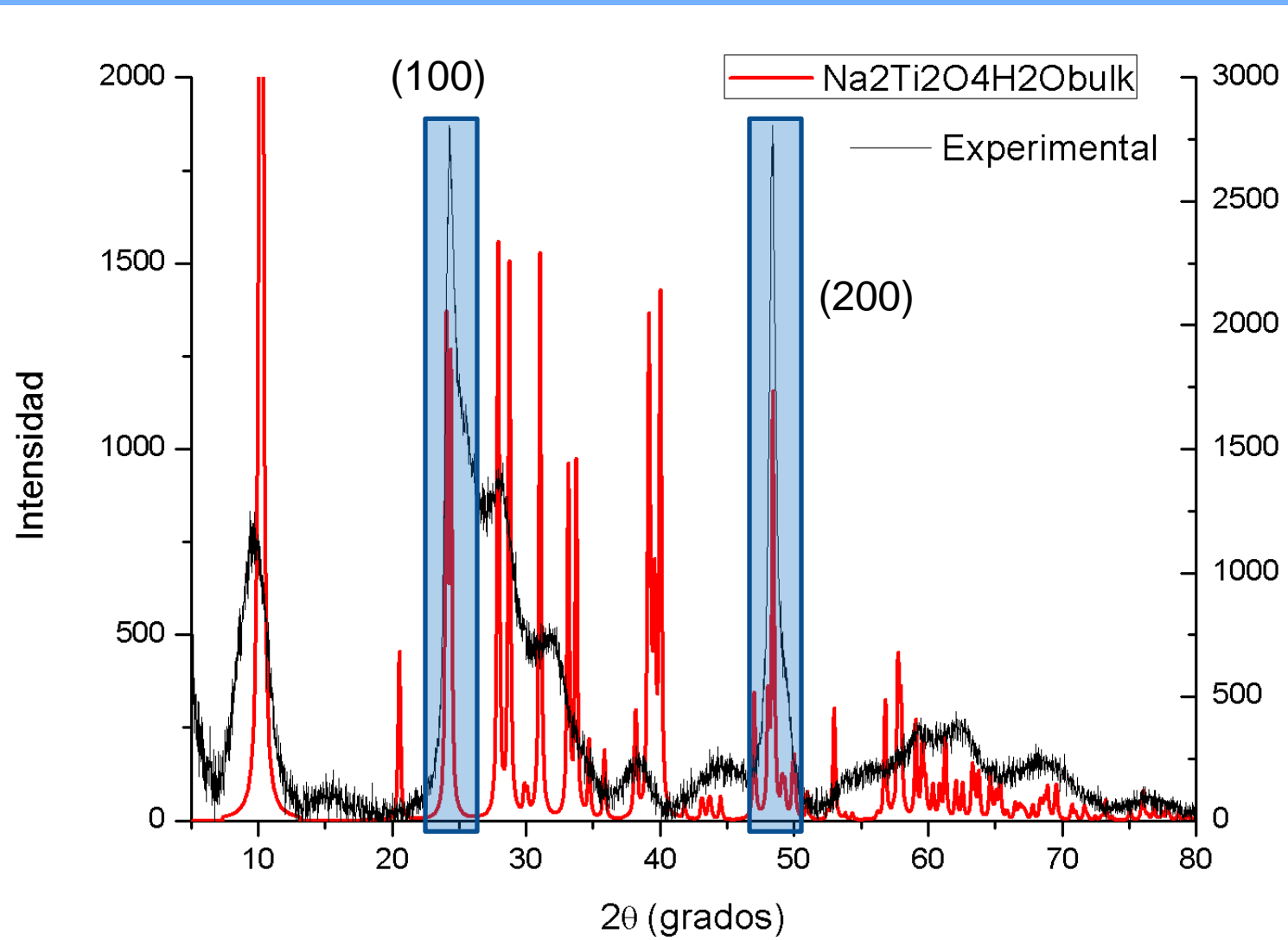


Bragg-Brentano focusing geometry (BB) Parallel beam geometry (PB)

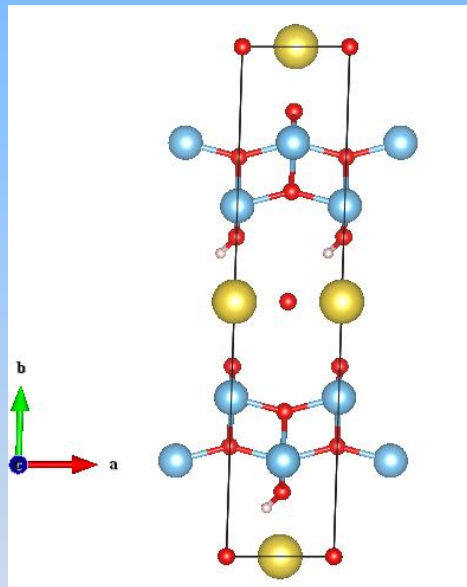


Rigaku

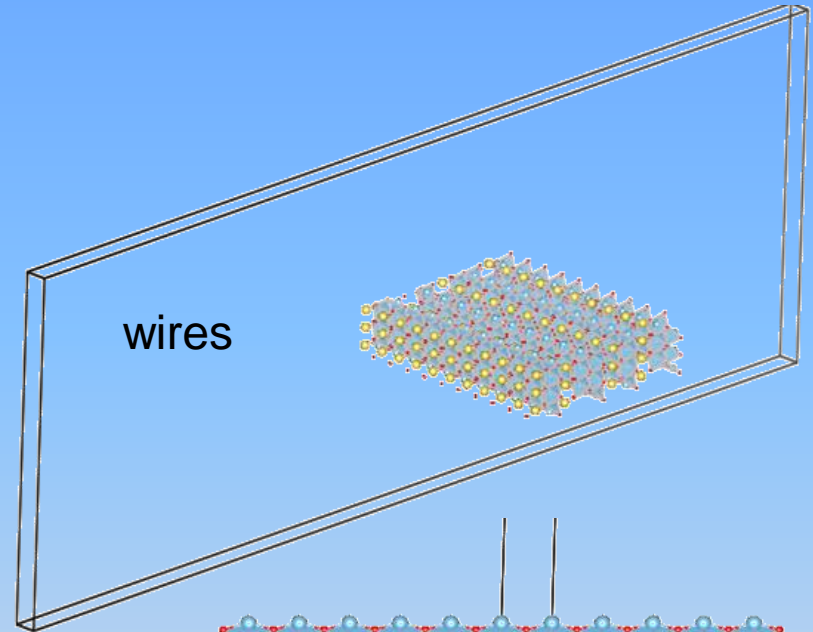
XRD Convencional



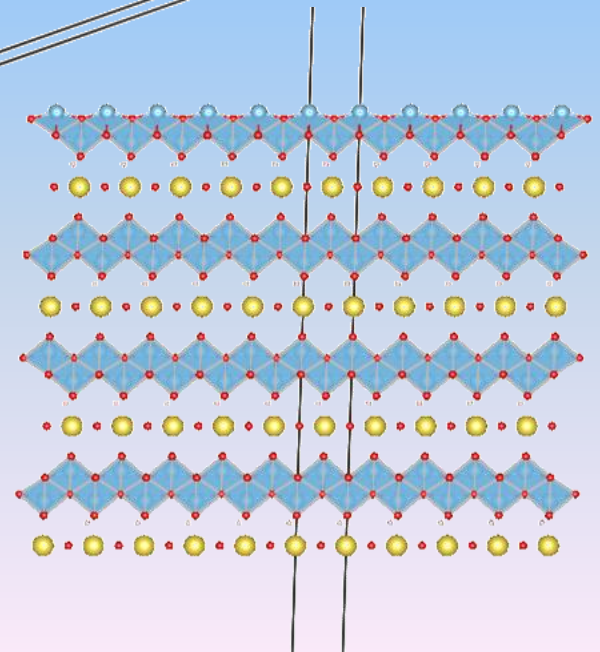
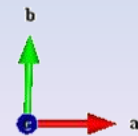
4- Bloques de construcción



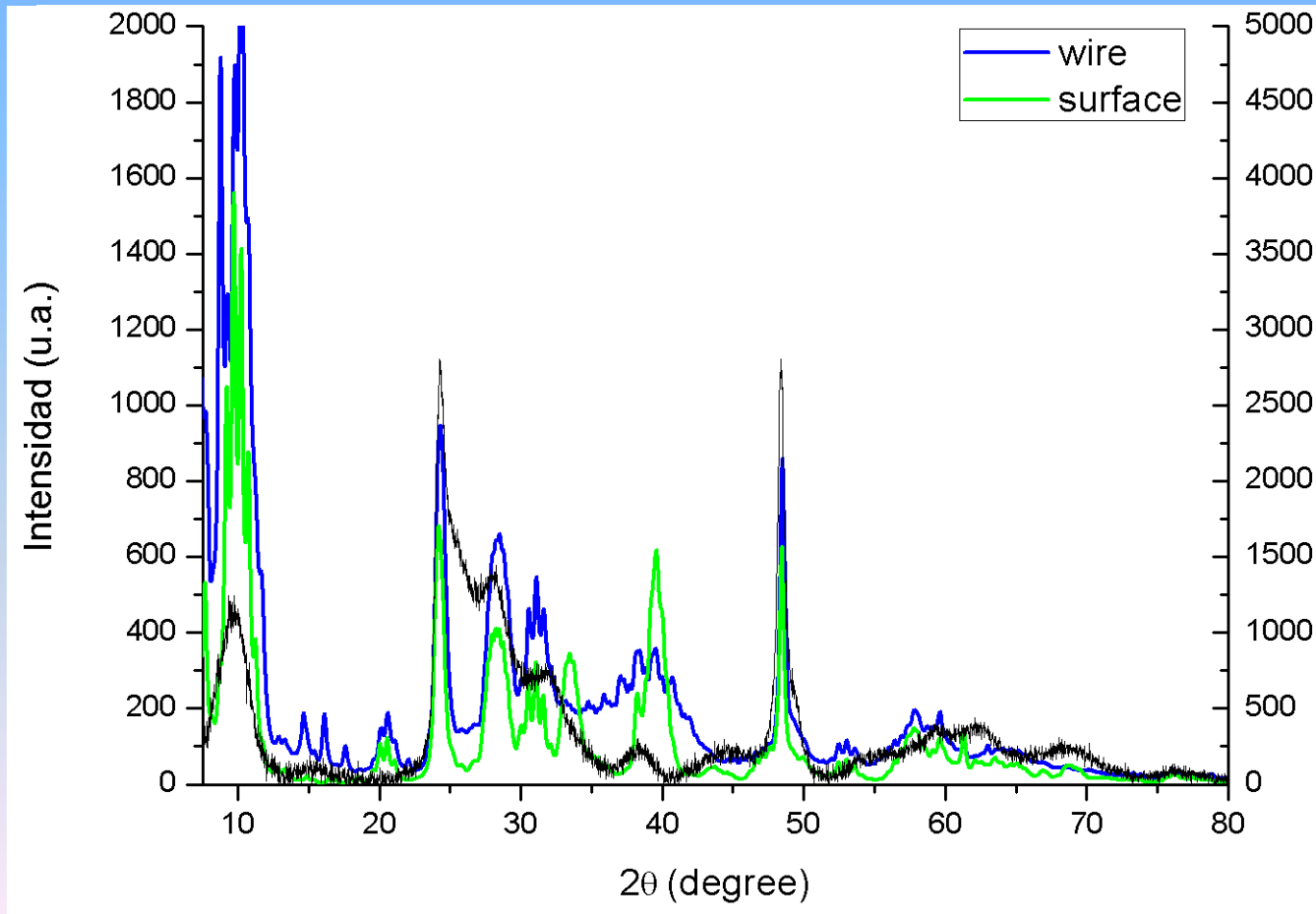
bulk



slabs

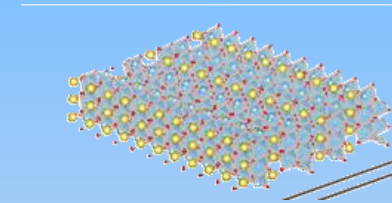
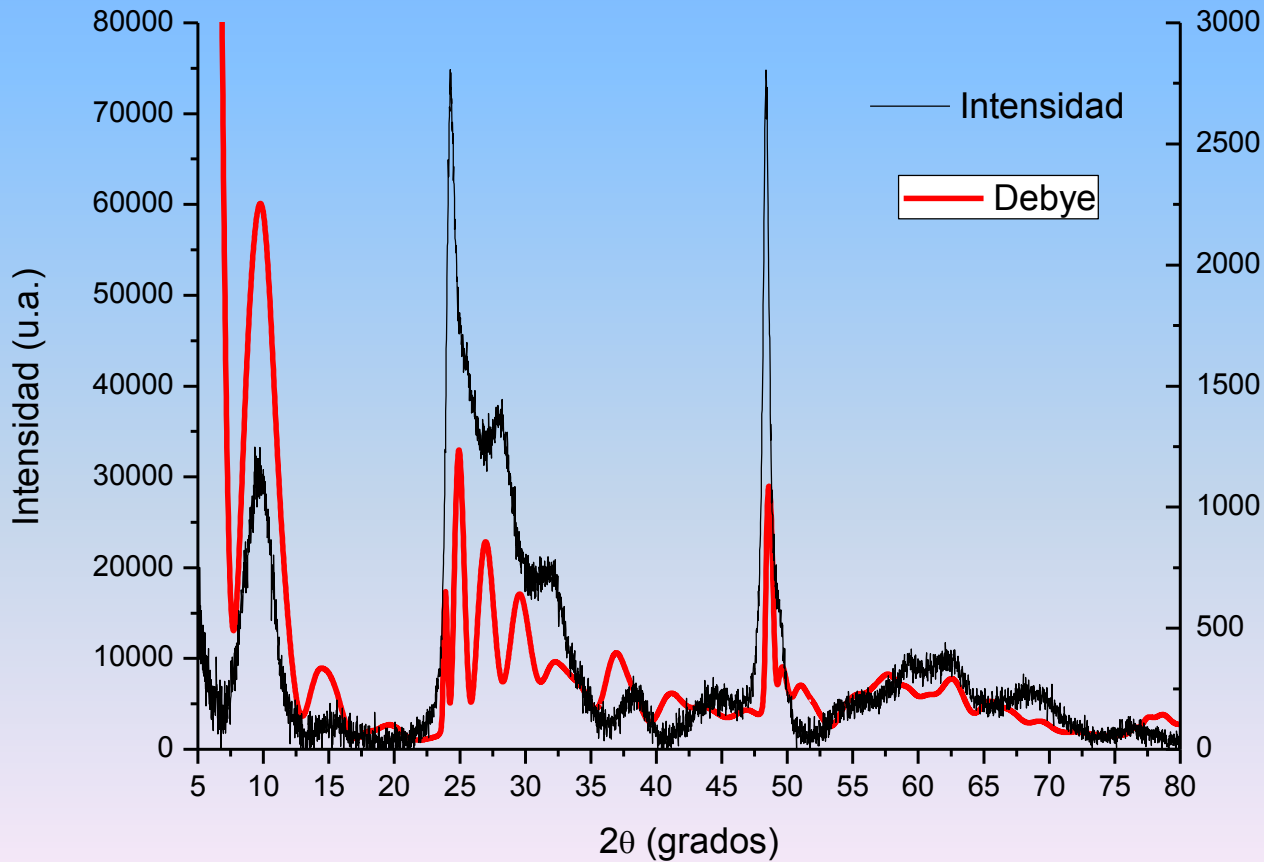


Ajustes globales de perfil: Rietveld



Debye Fitting:

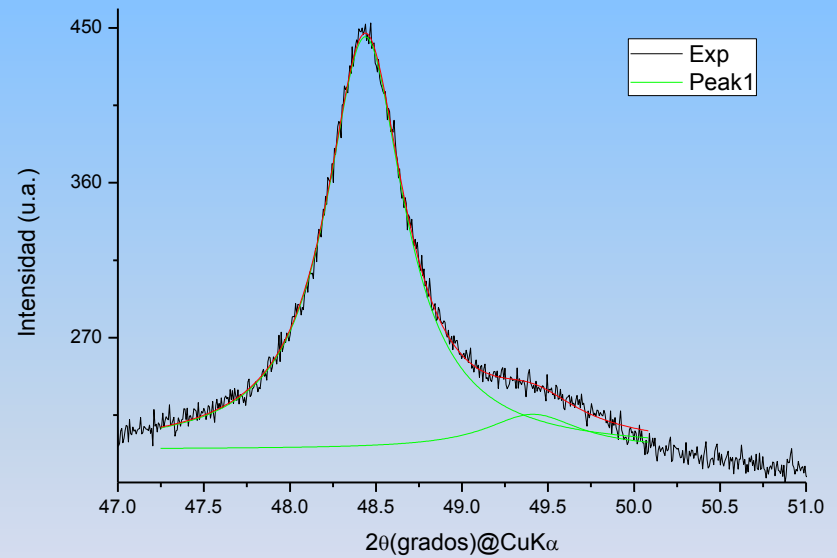
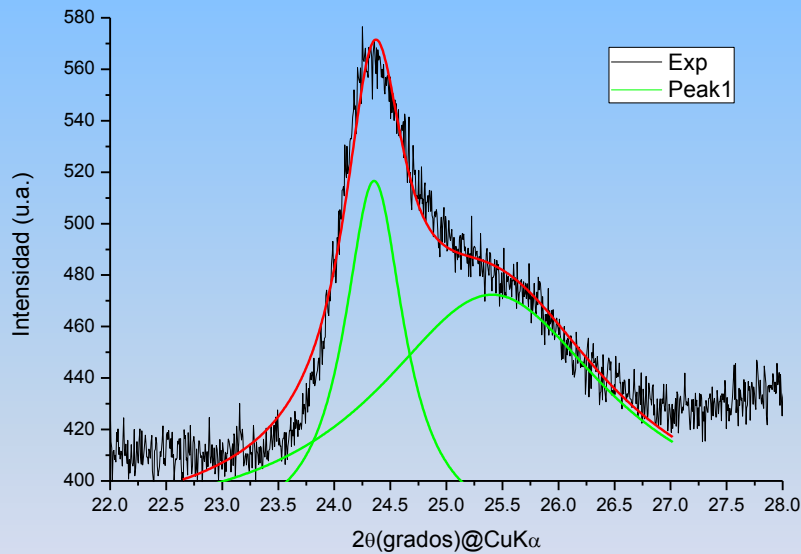
$$I_m(q) = \sum_{j=1}^{N_A} \sum_{i=1}^{N_A} f_i(q) f_j(q) \frac{\sin(qd_{ij})}{qd_{ij}}$$



$a=35.466 \text{ \AA} \quad \times 1$
 $b=3.757 \text{ \AA} \quad \times 300$
 $c=9.759 \text{ \AA} \quad \times 5$

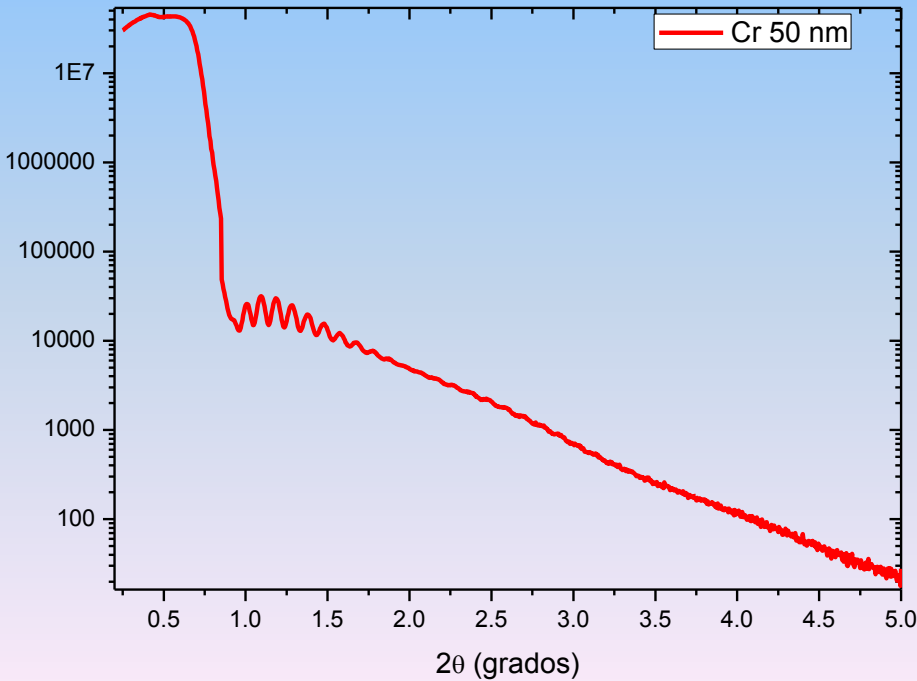
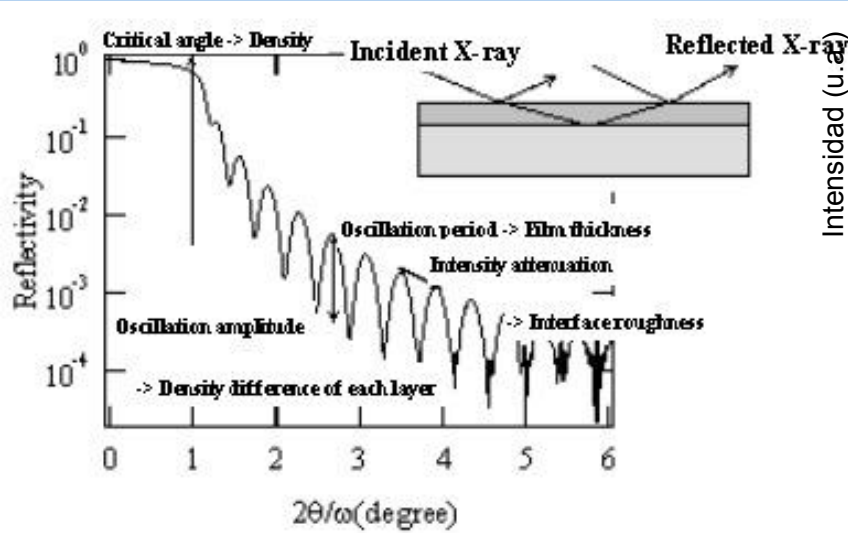
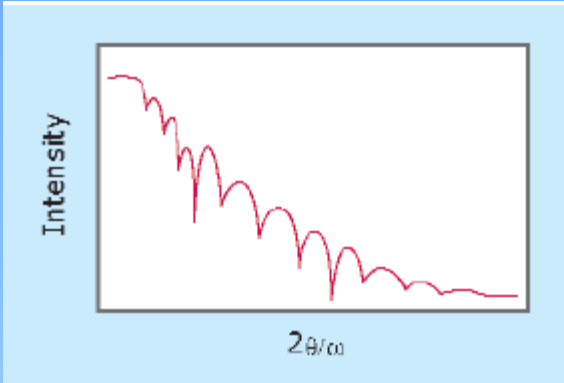
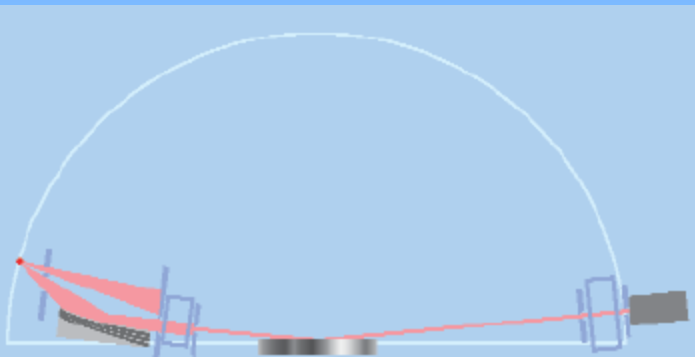


Scherrer Peak fitting



tamaño 19.2 14.9 nm

XRR: Reflectometria



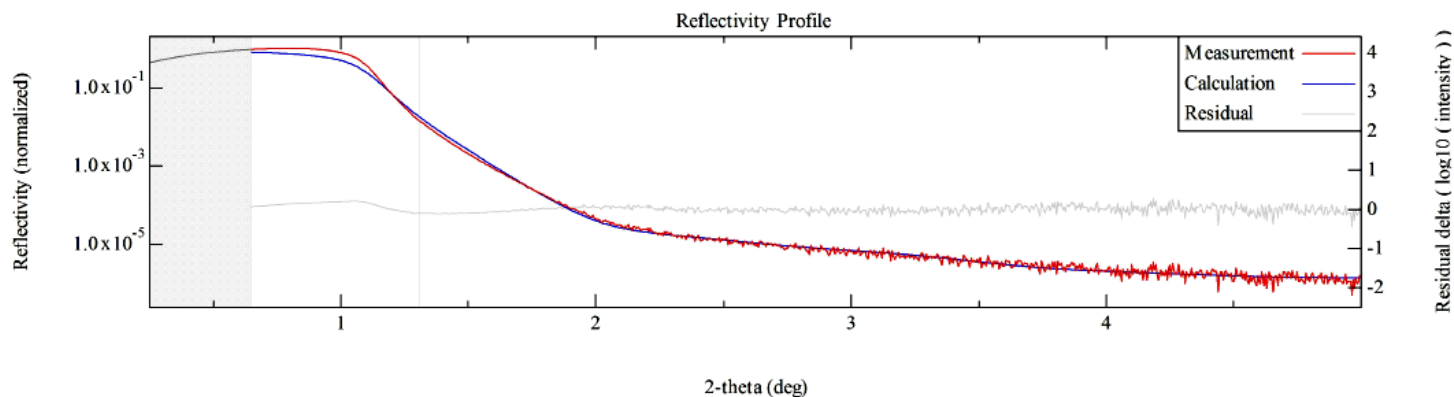
- XRR de capa fina de Au

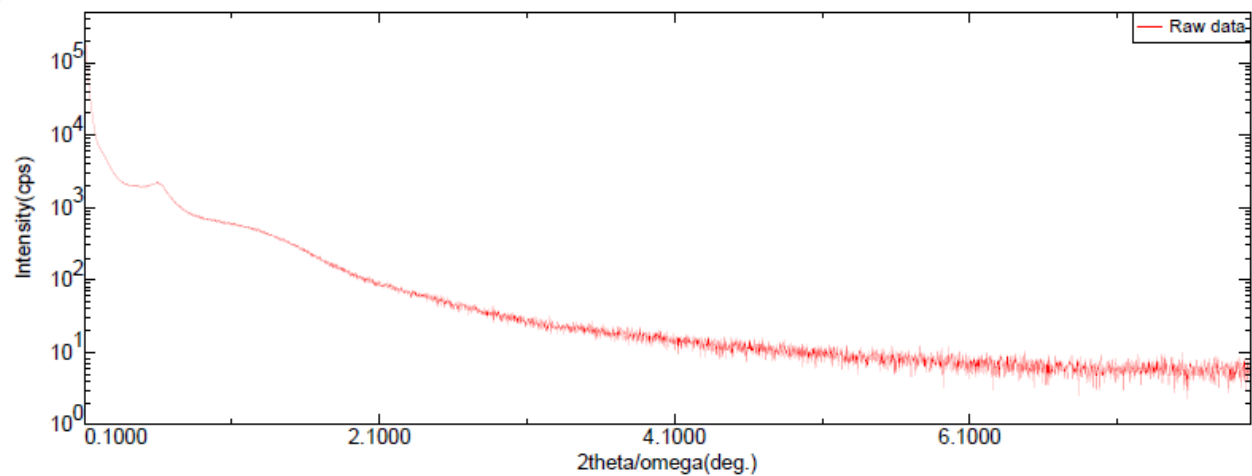
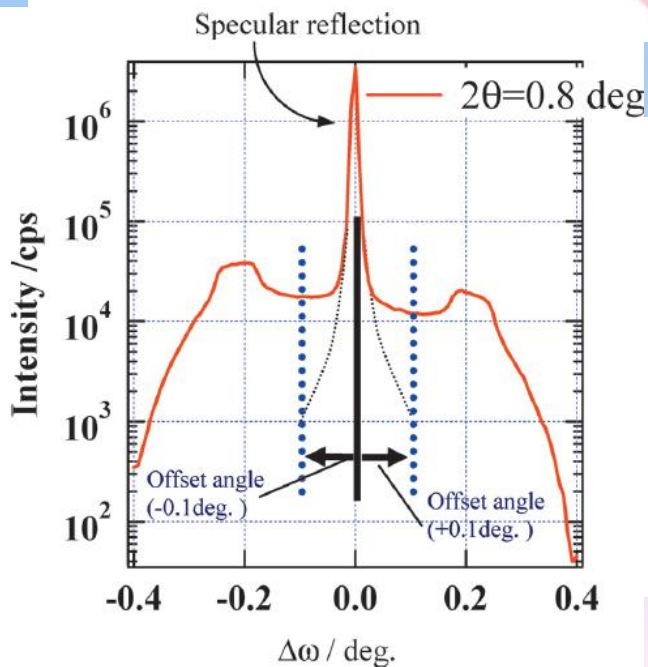
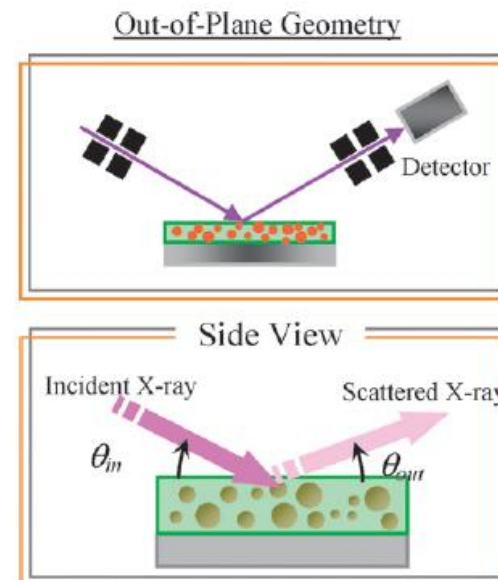
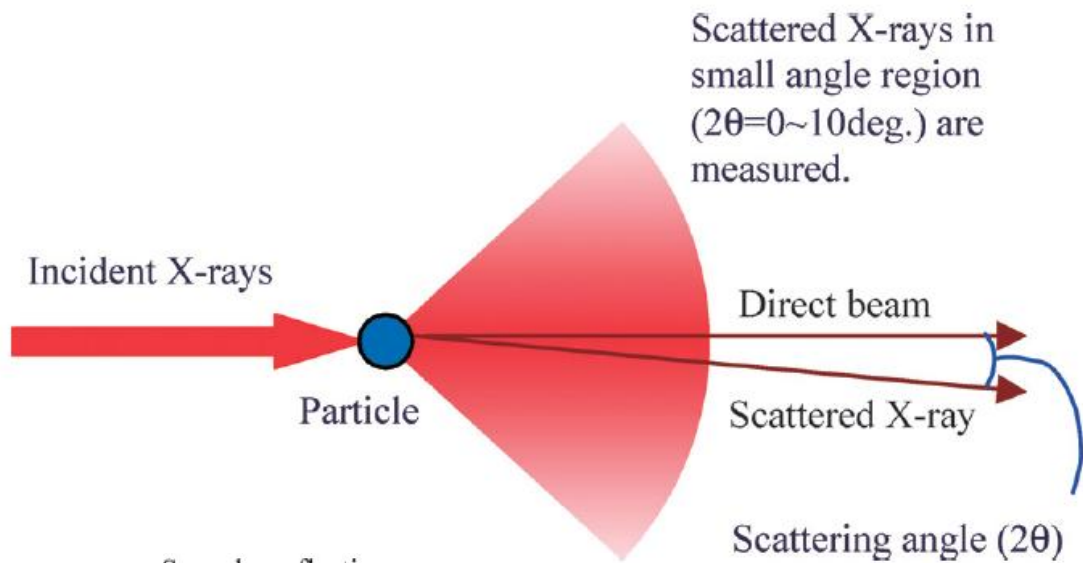
Layername: Au
 Thickness: 103.7(12)nm
 Density: 18.73(10)
 Roughness: 1.861(8)

Layername: Cr
 Thickness: 8.48(16)nm
 Density: 2.68(12)

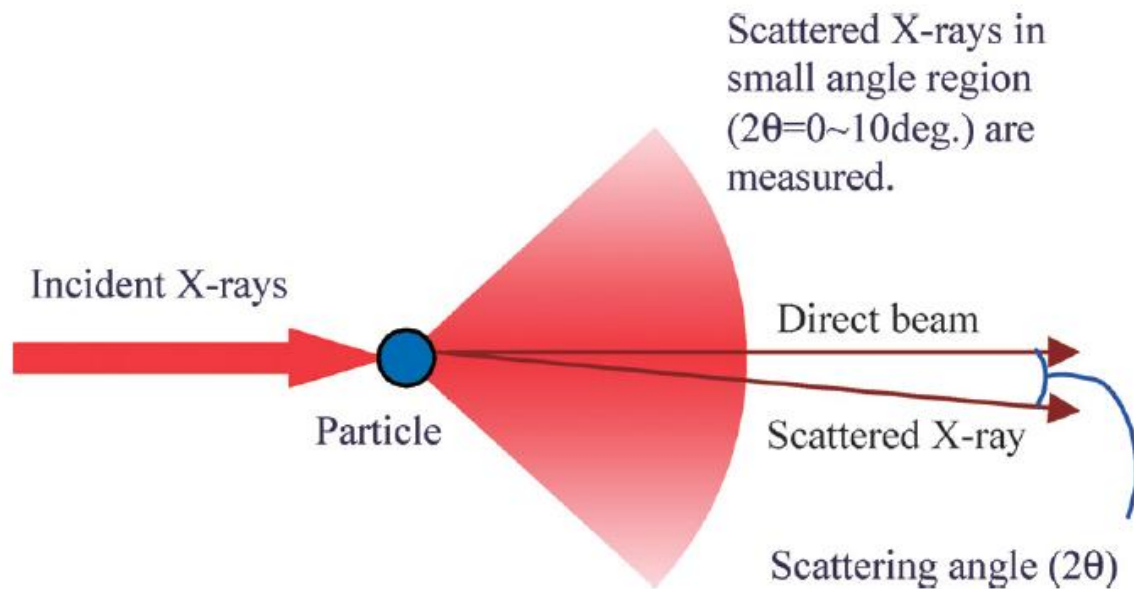
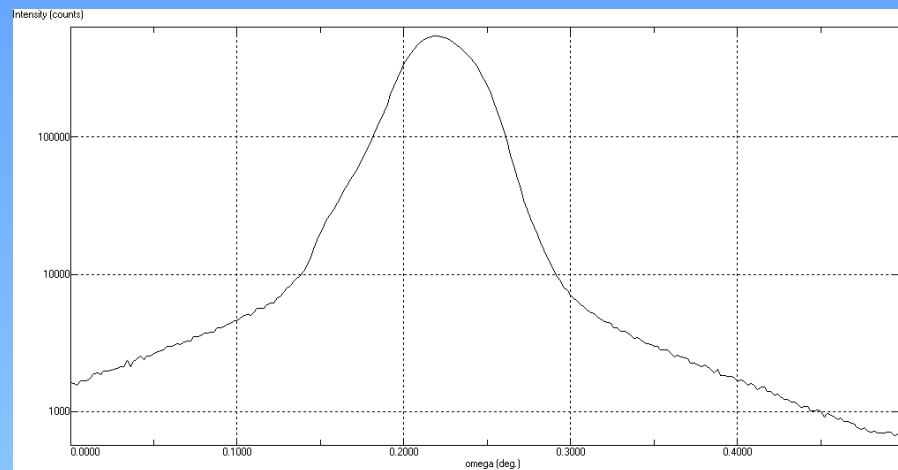
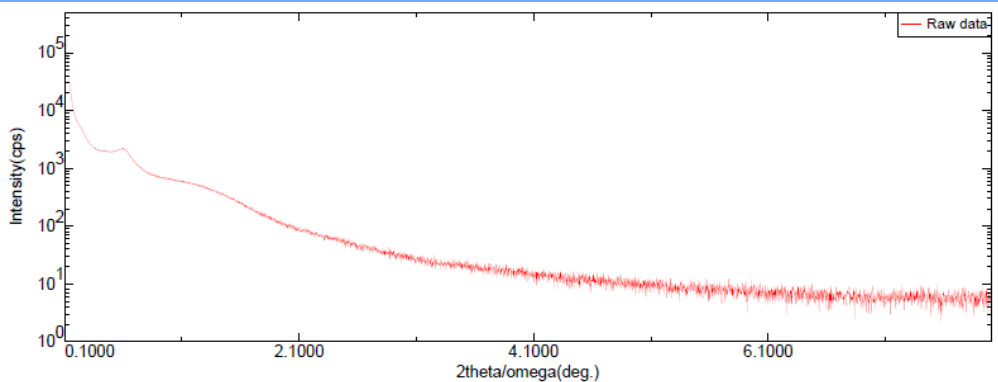
Substrate name: GLASS
 Density: 2.21
 Roughness: 0.50

ID	Material	Thickness (nm)	Density (g/cm3)	Roughness (nm)
2	Au	103.7(12)	18.73(10)	1.861(8)
1	Cr	8.48(16)	2.68(12)	0.684(7)
Sub.	GLASS	0.0[--]	2.21[--]	0.50[--]

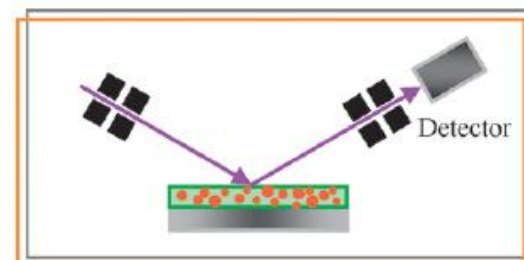




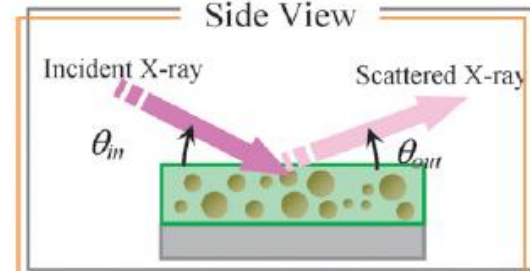
Rocking Curve



Out-of-Plane Geometry

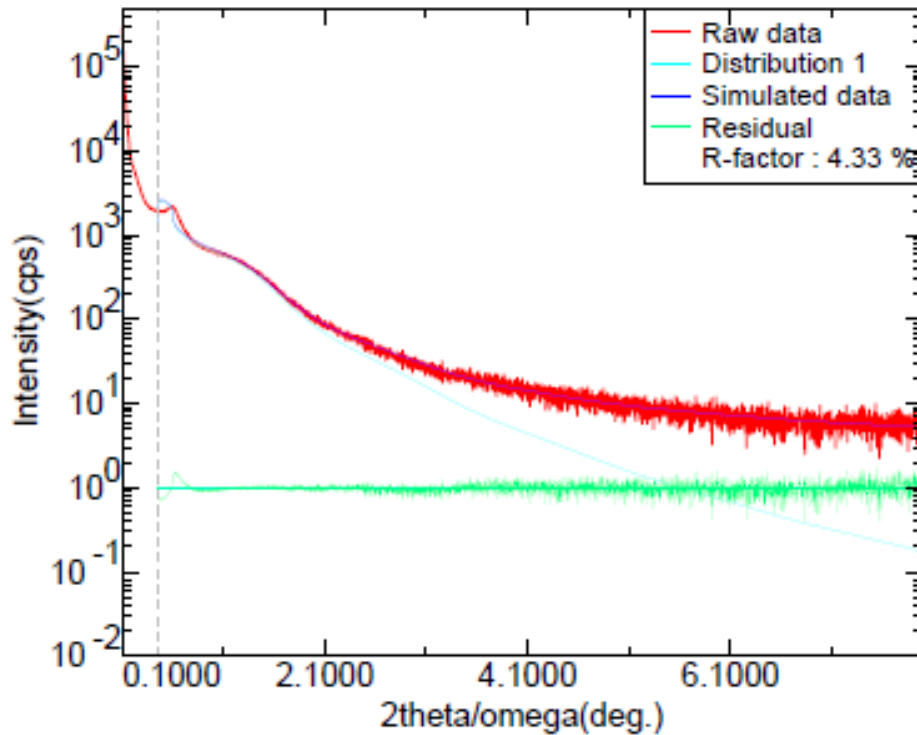


Side View



SAXS reflectometria

Particle-/Pore-size Analysis



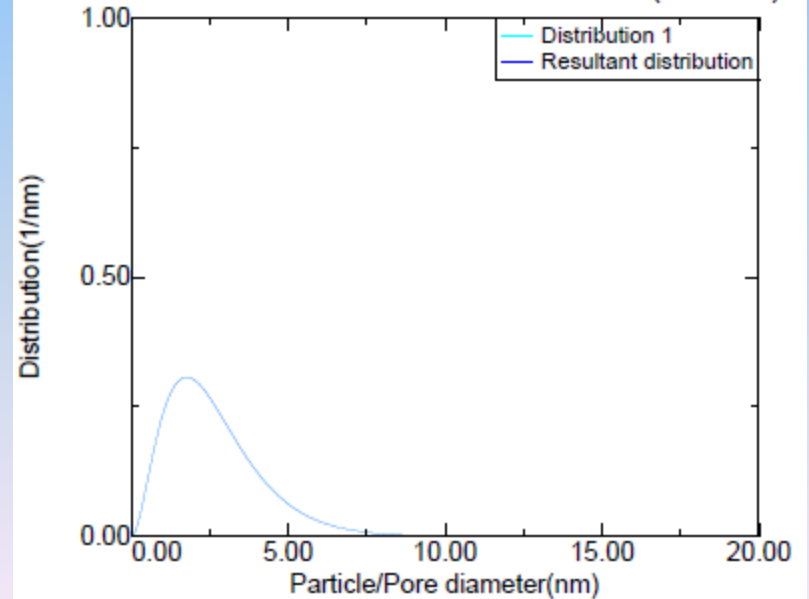
Sample name : NT TiO₂

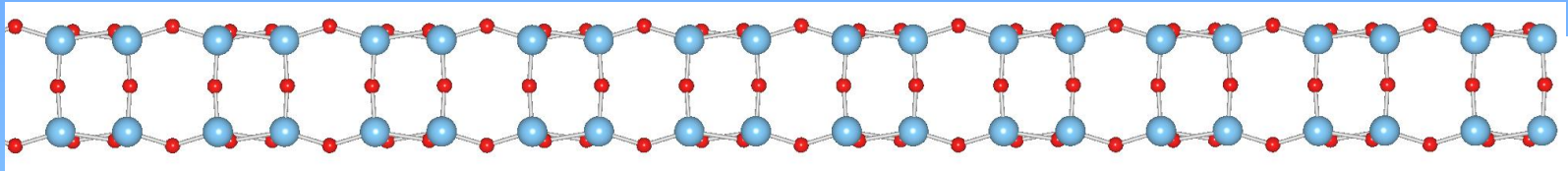
Comment :

Distribution	Average diam (nm)	Aspect Ratio	Norm. disp. (%)	Scale (1.000E+010)	Nearest (nm)	Pack. fr.(%)	Volume (%)
1	2.647	[10.00]	57.7	0.0782	5.819	22.24	100.00
	2.64	10.0	57.7%		5.819	22.24	

BG function : 1/sin(theta) R-factor : 4.33 %
 BG : 4.96 Average diam. : 2.647 nm

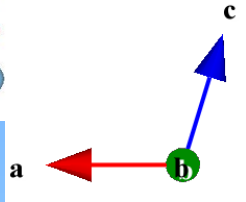
Particle-/Pore-size Distribution(Volume)



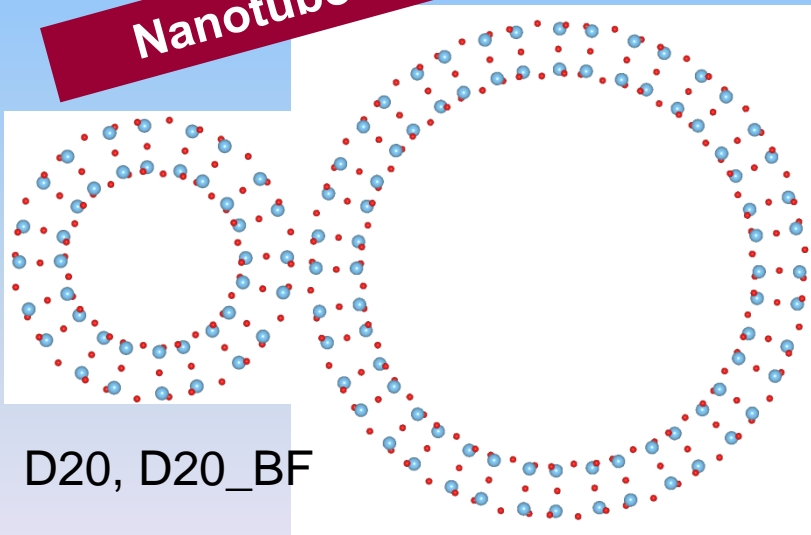


Modelos unidimensionales iniciales

$$x' = (R - z) \cos\left(\frac{x}{R}\right) \quad z' = (R - z) \operatorname{sen}\left(\frac{x}{R}\right)$$



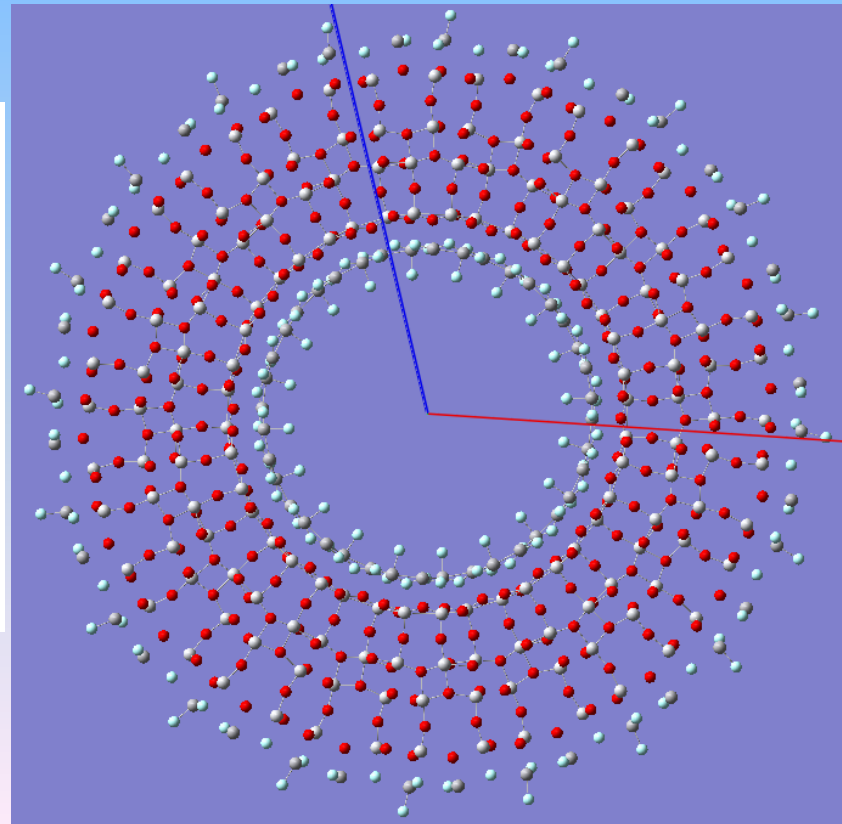
Nanotubos



D20, D20_BF

D40, D40_BF

D40_DW_BF

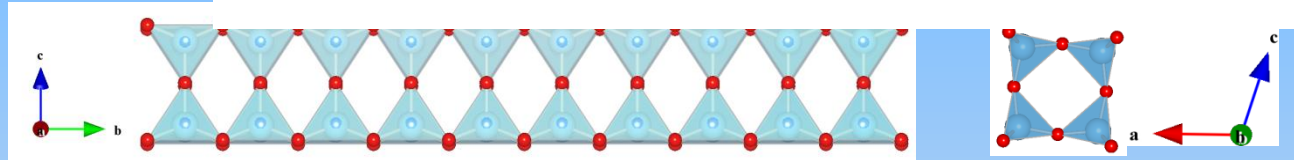


Selección de Bloques

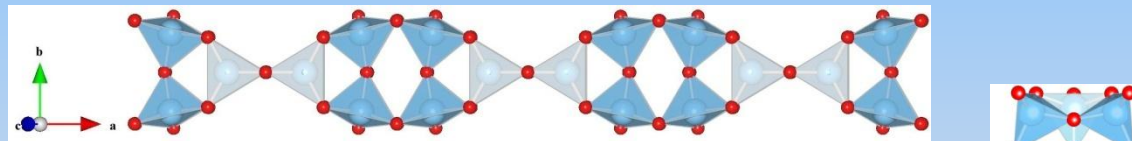
Reconstrucción estructural

WIRE	N° átomos	E (eV/TiO ₂)	CV	p(Å)	$\Delta p(\%)$	ΔE_{bulk} (eV/TiO ₂)	$\Delta E_{\text{bulk, A}}$ (eV/TiO ₂)	GAP (eV)
<u>TB_wire_x</u>	36	-970.13	No	12.18	---	0.62	0.55	
	36	-970.17	Sí	11.55	5.2	0.57	0.51	2.99
<u>TB_wire_y</u>	12	-969.68	No	3.74	---	1.07	1.00	
	12	-970.41	Sí	3.18	15.1	0.33	0.27	3.47
<u>TB_wire_200_z</u>	12	-970.02	No	6.55	---	0.73	0.66	
	12	-970.03	Sí	6.43	1.8	0.72	0.65	3.53
<u>A_wire_z</u>	27	-969.80	No	9.51	---	0.88	0.88	
	27	-969.80	Sí	9.49	0.2	0.88	0.88	3.21

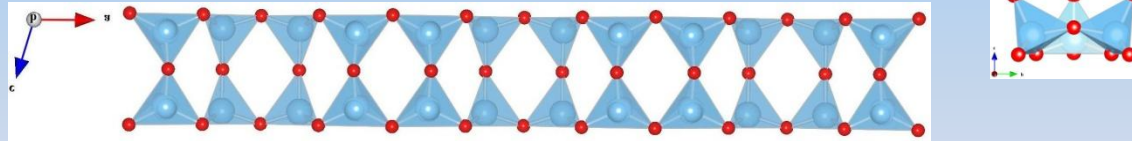
TB_wire_y



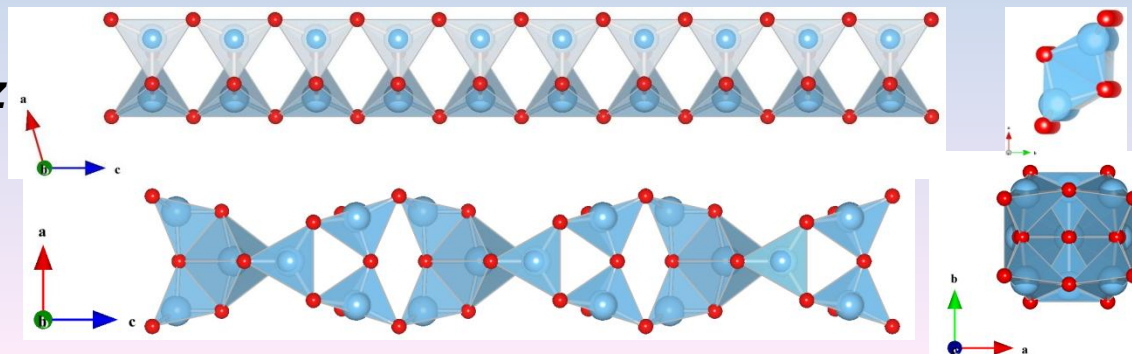
TB_wire_x



TB_wire_200_z



A_wire_z



Muchas gracias

