

Sociedad Mexicana
de Materiales A.C.

CAPÍTULOS ESTUDIANTILES SMM

TALLER DE ESPECTROSCOPIA DE ELECTRONES FOTOEMITIDOS (XPS).

Mariela Bravo Sánchez
Universidad de Guadalajara

08 de noviembre de 2018

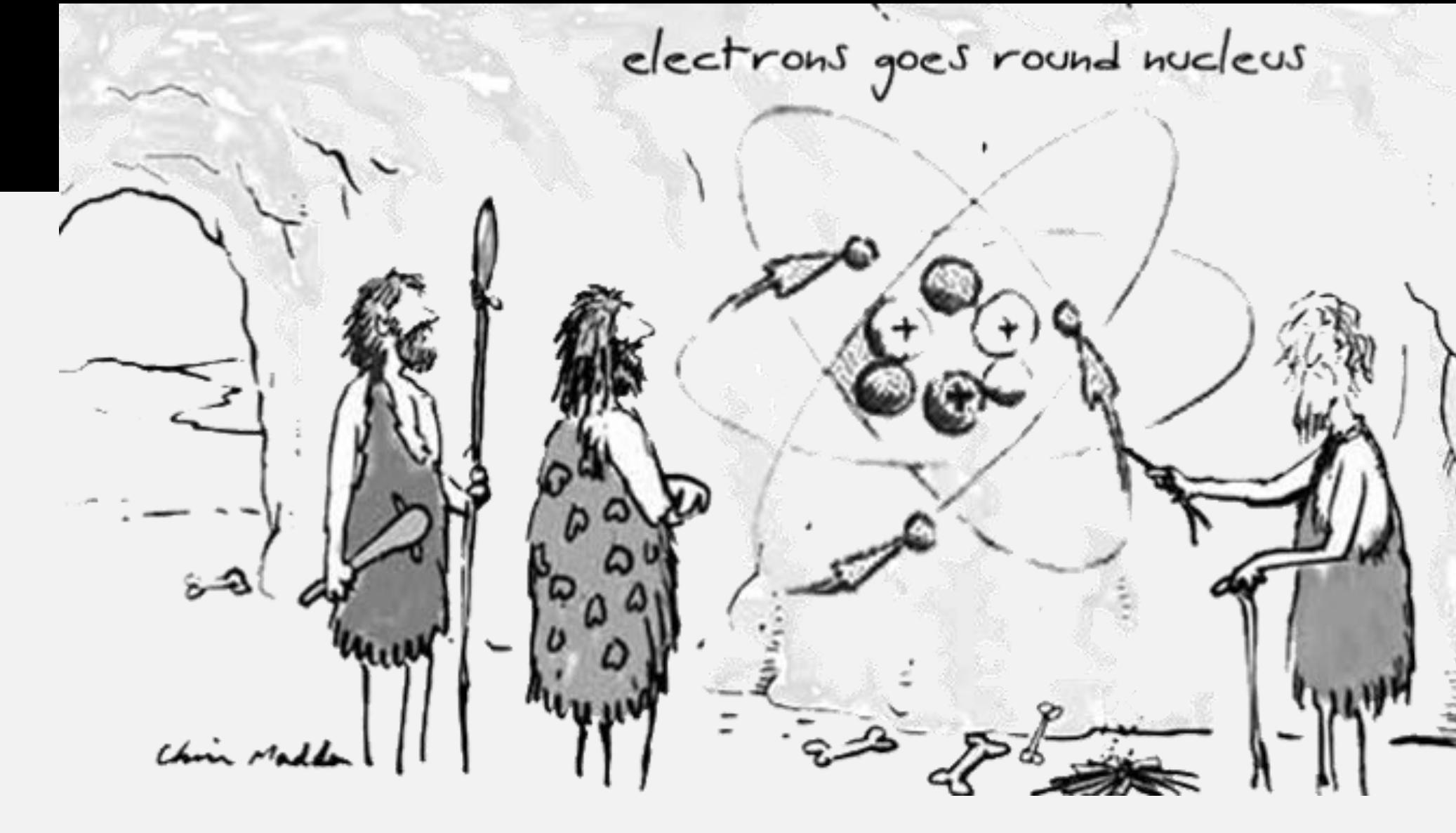


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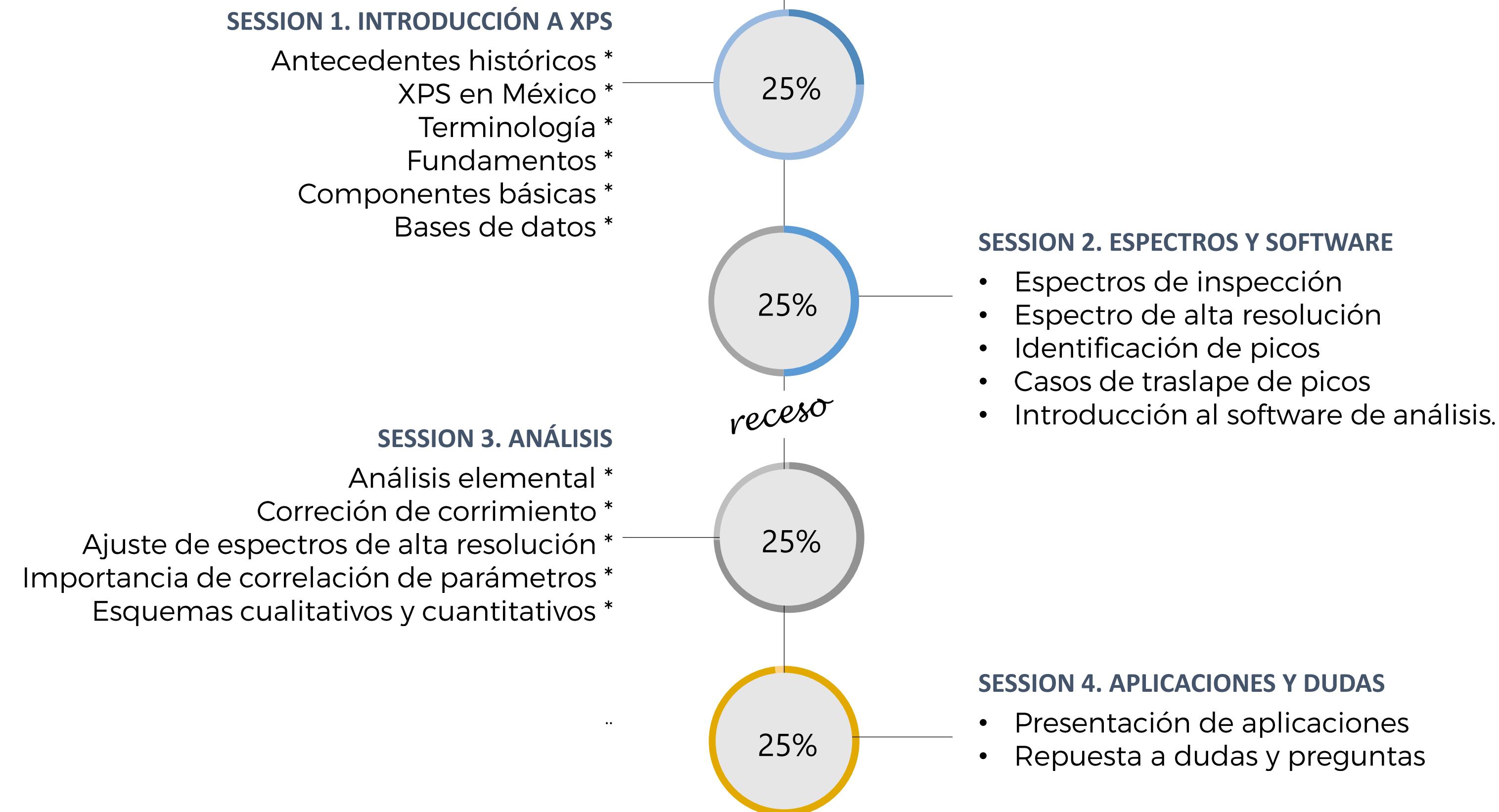
ESPECTROSCOPIA DE ELECTRONES FOTOEMITIDOS X-RAY PHOTOELECTRON SPECTROSCOPY (XPS)

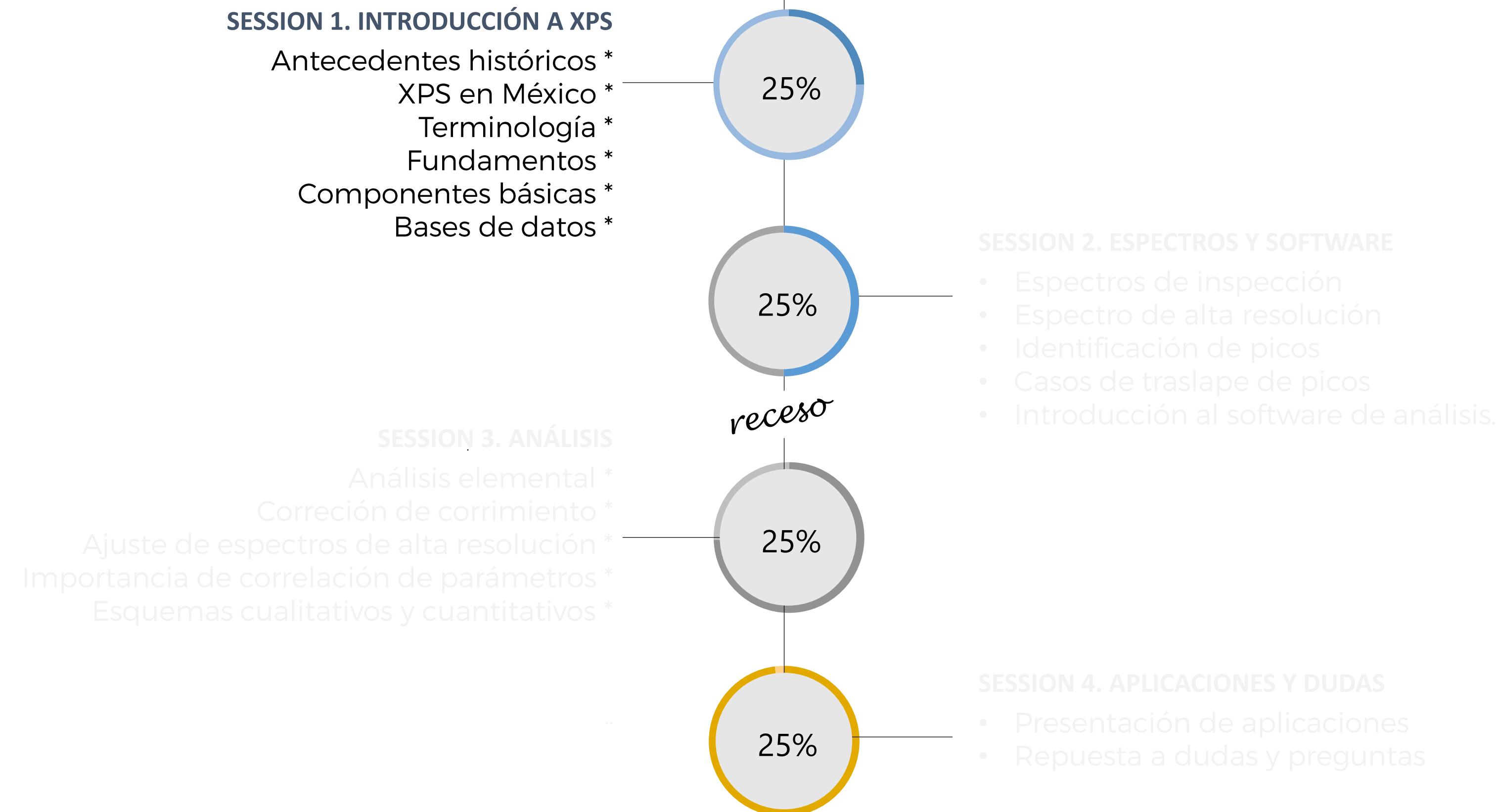


XPS es una herramienta de caracterización química utilizada para **cuantificar elementos** y **estados de oxidación** presentes en la superficie de los materiales. En este taller se abordarán los principios **fundamentales** de la técnica, las componentes del sistema, adquisición de datos y el análisis **cualitativo/cuantitativo** tanto elemental como de estados químicos y se ilustrará su utilidad en alguna **aplicaciones**.

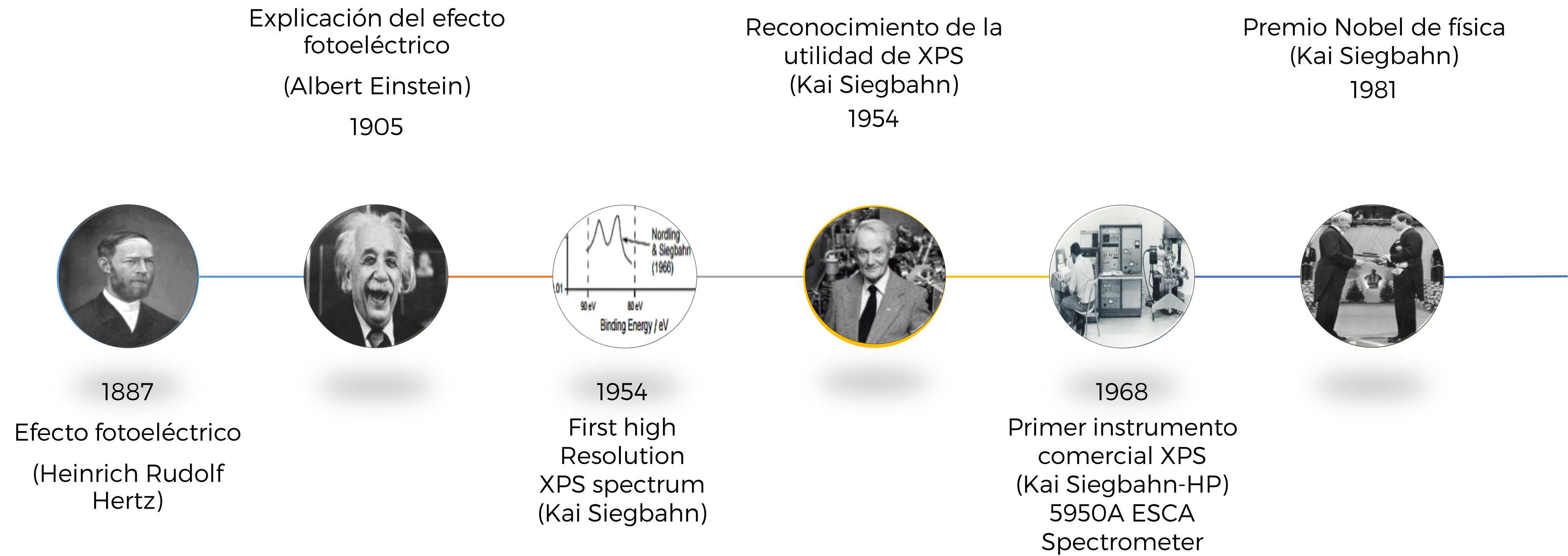
Al final del curso:

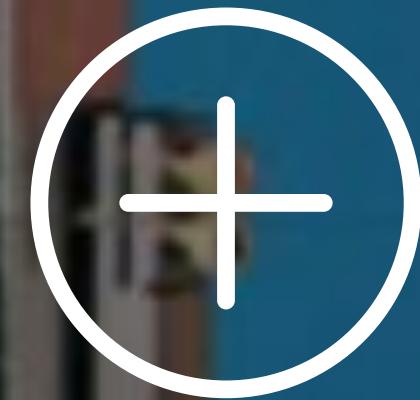
- Conocerás los principios físicos y técnicos fundamentales de XPS.
- Conocerás las herramientas básicas para realizar el análisis como son, software y bases de datos.
- Comprenderás su utilidad para en análisis químico superficial en distintas aplicaciones





Time, it flies when you're busy





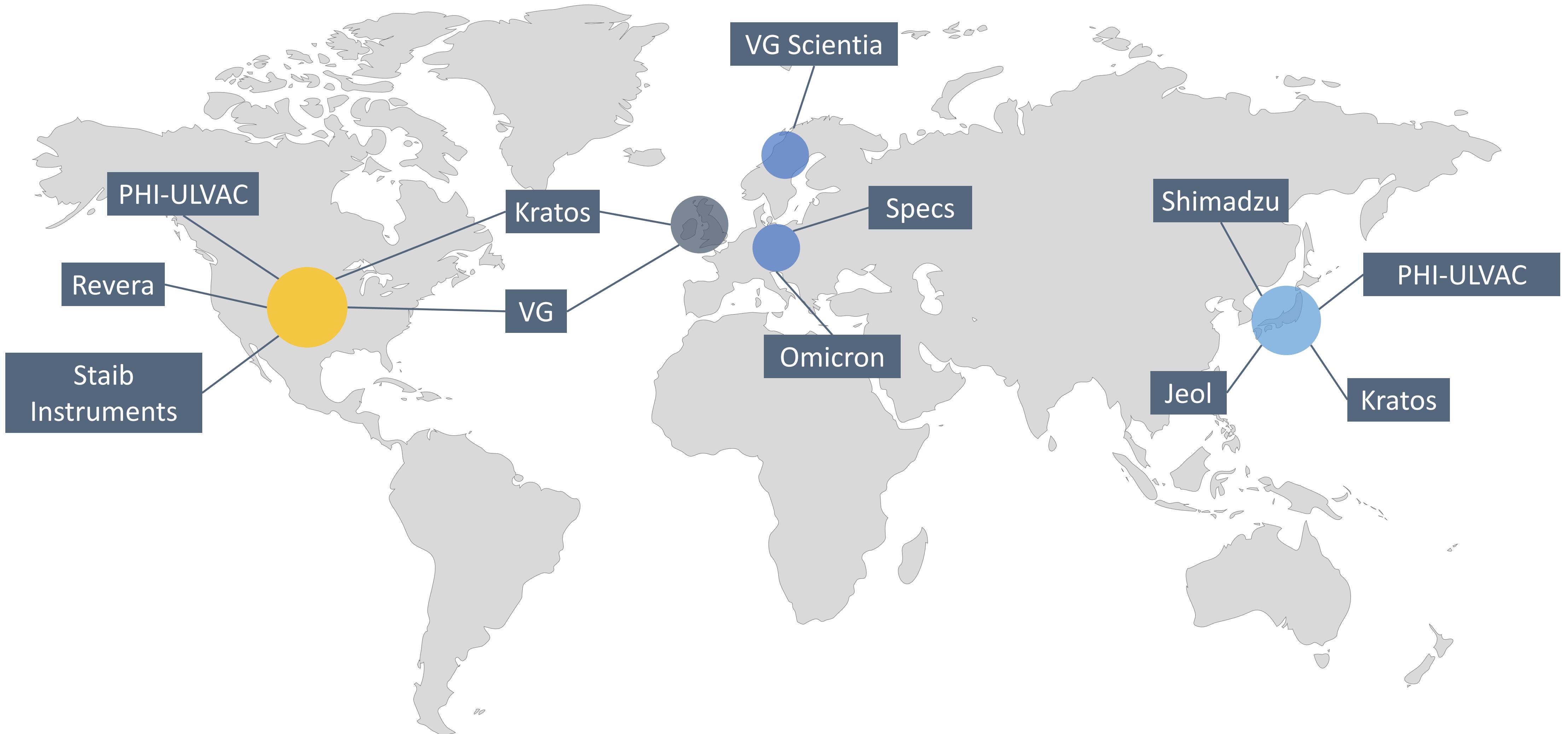
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Siegbahn and his colleagues pursued this technique calling it ESCA (Electron Spectroscopy for Chemical Analysis), and have published numerous papers and two excellent books describing their researches. HP became interested in the technique in 1968 at the instigation of the member of the board of directors, Luis Alvarez, and Don Hammond, the director of Physical Electronics Laboratory. They saw that the technique had great potential, both as a general-purpose research tool and as analytical instrument to solve applied problems. A development project was initiated in the Physical Electronics Laboratory with Professor Siegbahn as consultant and the result was the Model 5950A ESCA Spectrometer

PRINCIPALES FABRICANTES DE XP EN EL MUNDO

8



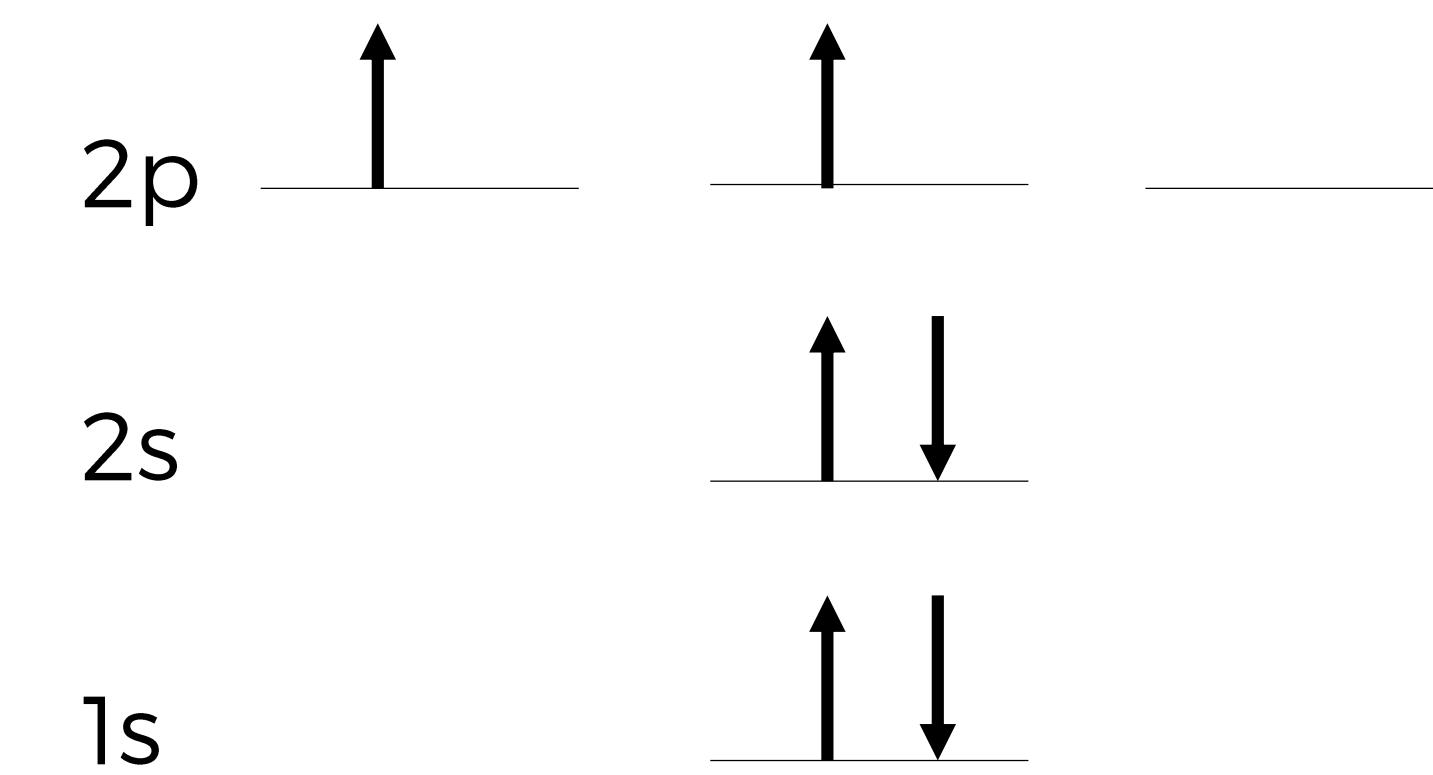
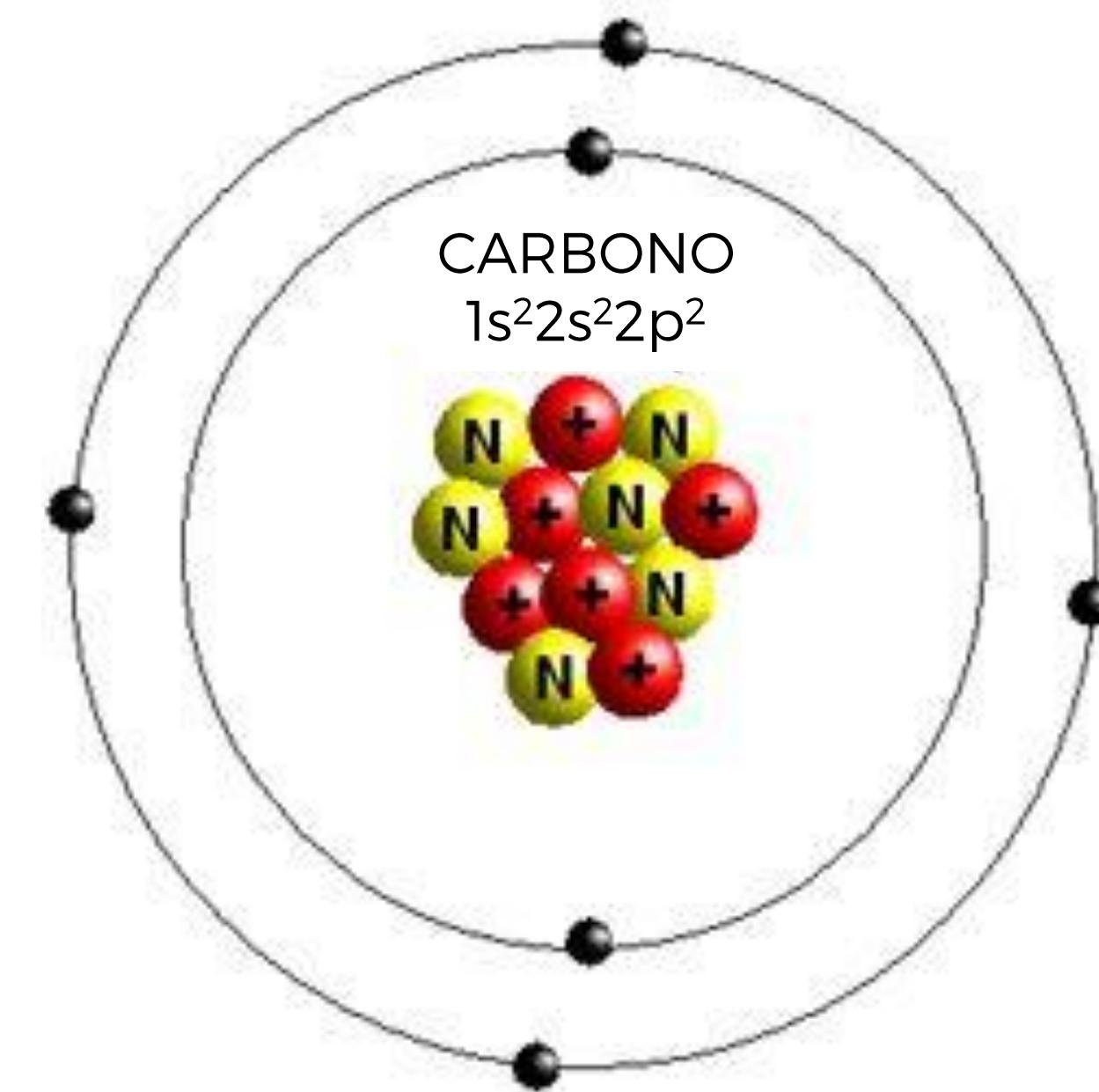
XPS EN MÉXICO

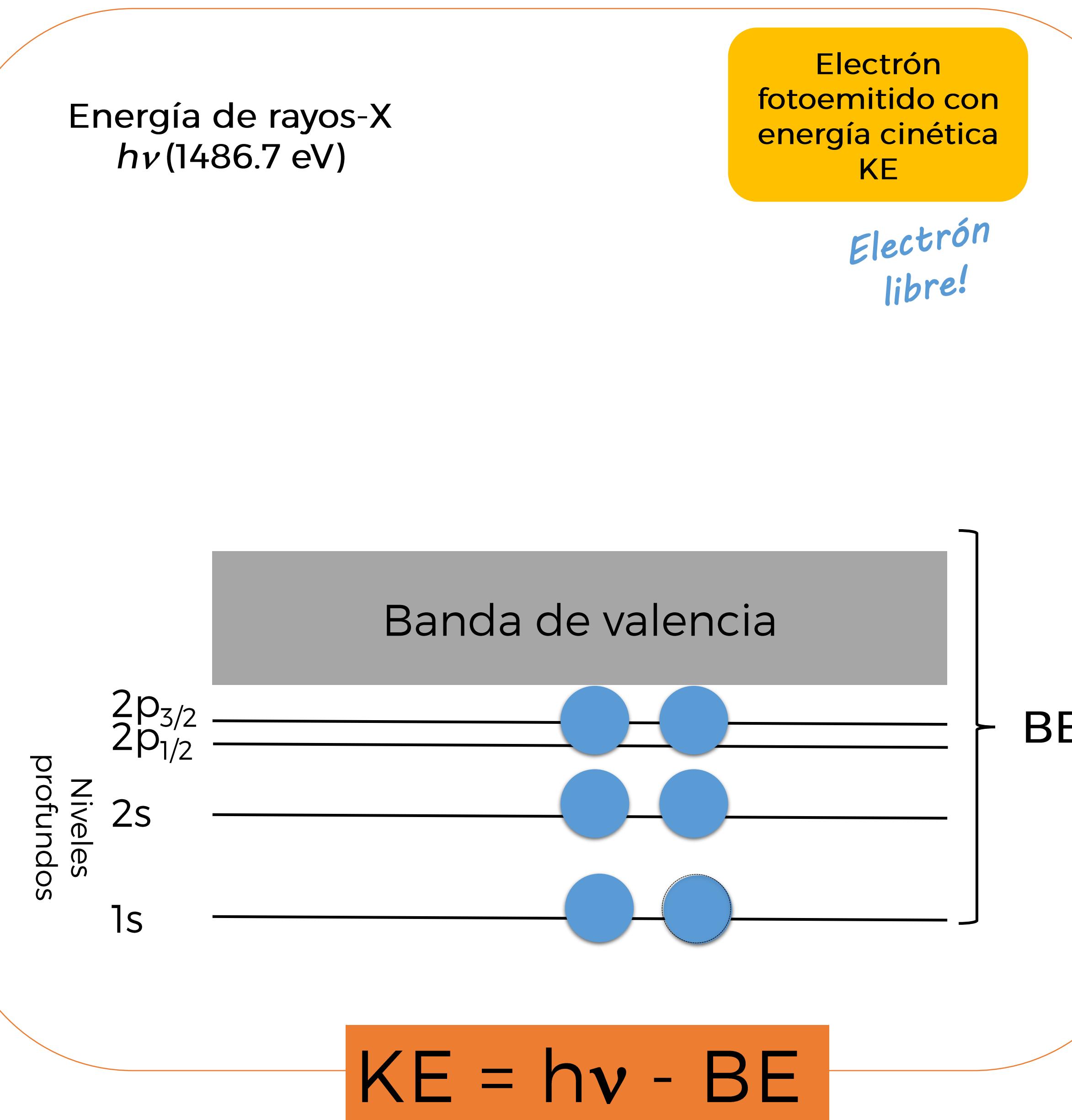
SISTEMAS XP EN MÉXICO

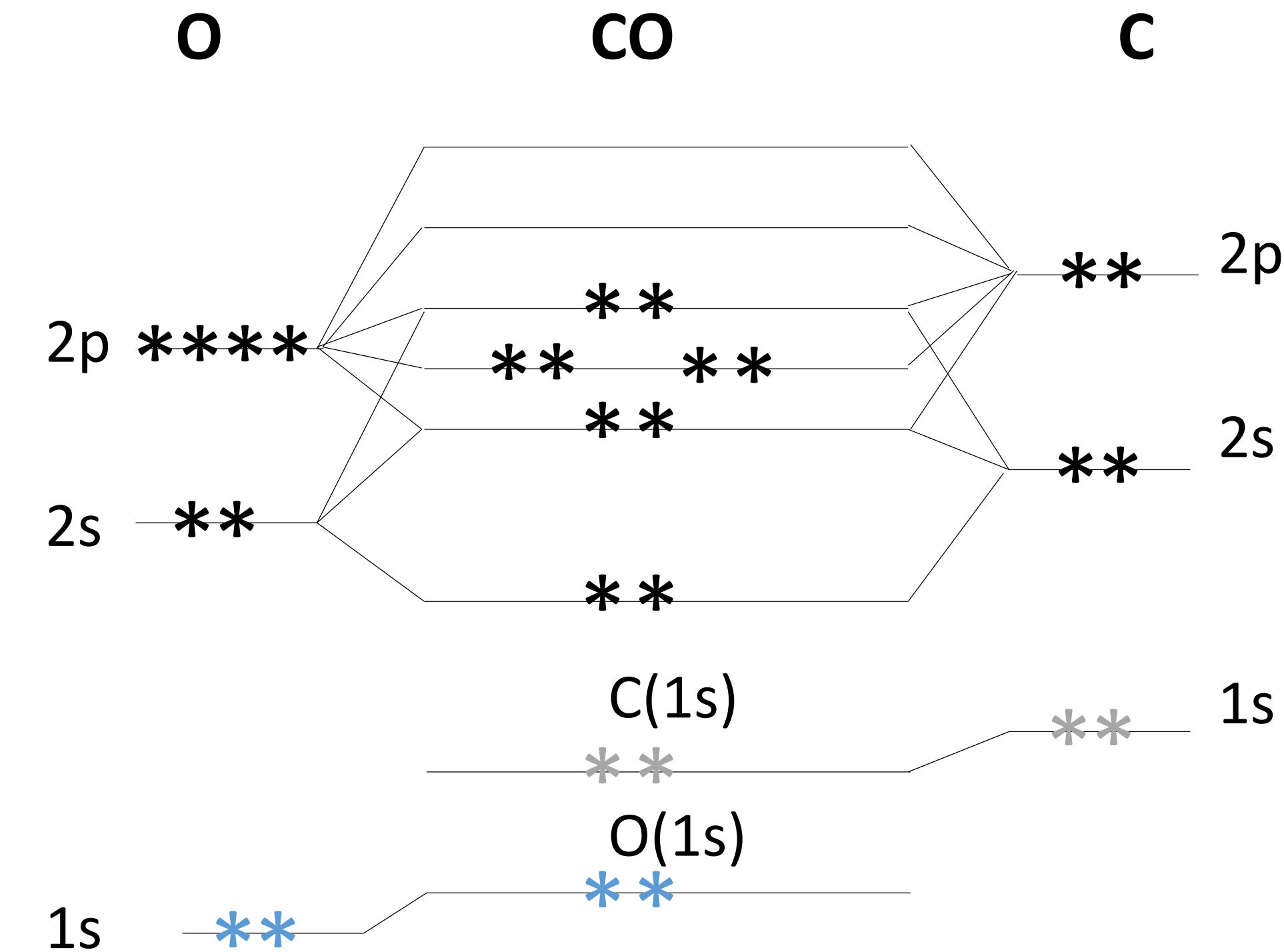
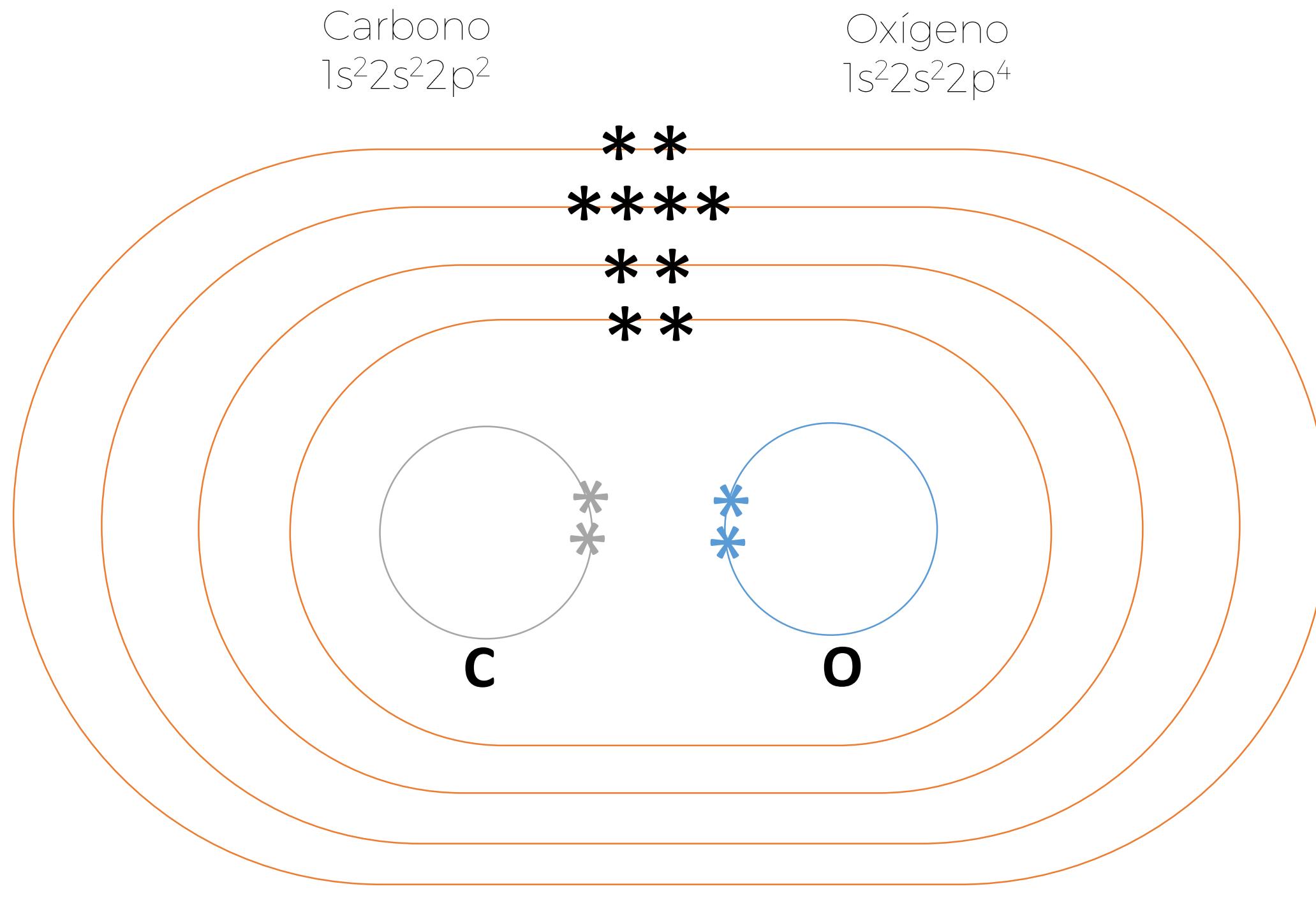


- ESCA - electron spectroscopy for chemical analysis
- XPS - X-ray photoelectron spectroscopy
- PES - photoemission spectroscopy
- HXPS or HAXPES - hard X-ray XPS
- ARXPS - angle-resolved XPS
- TRXPS - total reflection XPS
- NAPXPS - near ambient pressure XPS
- UPS - ultra-violet photoelectron spectroscopy
- AES - Auger electron spectroscopy

	1s	2s	2p	3s . . .
H	1			
He	2			
Li	2	1		
Be	2	2		
B	2	2	1	
C	2	2	2	
N	2	2	2	1

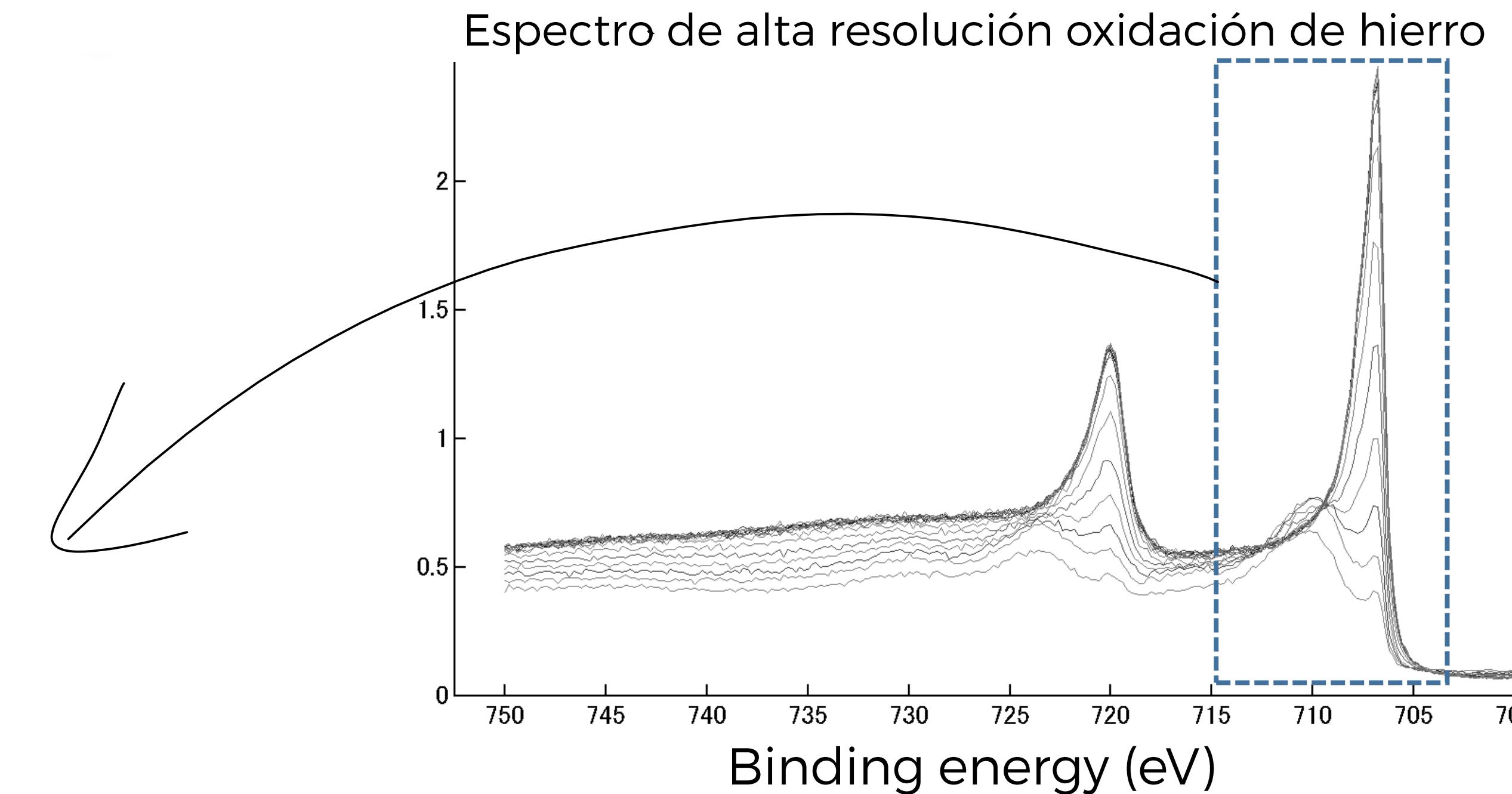
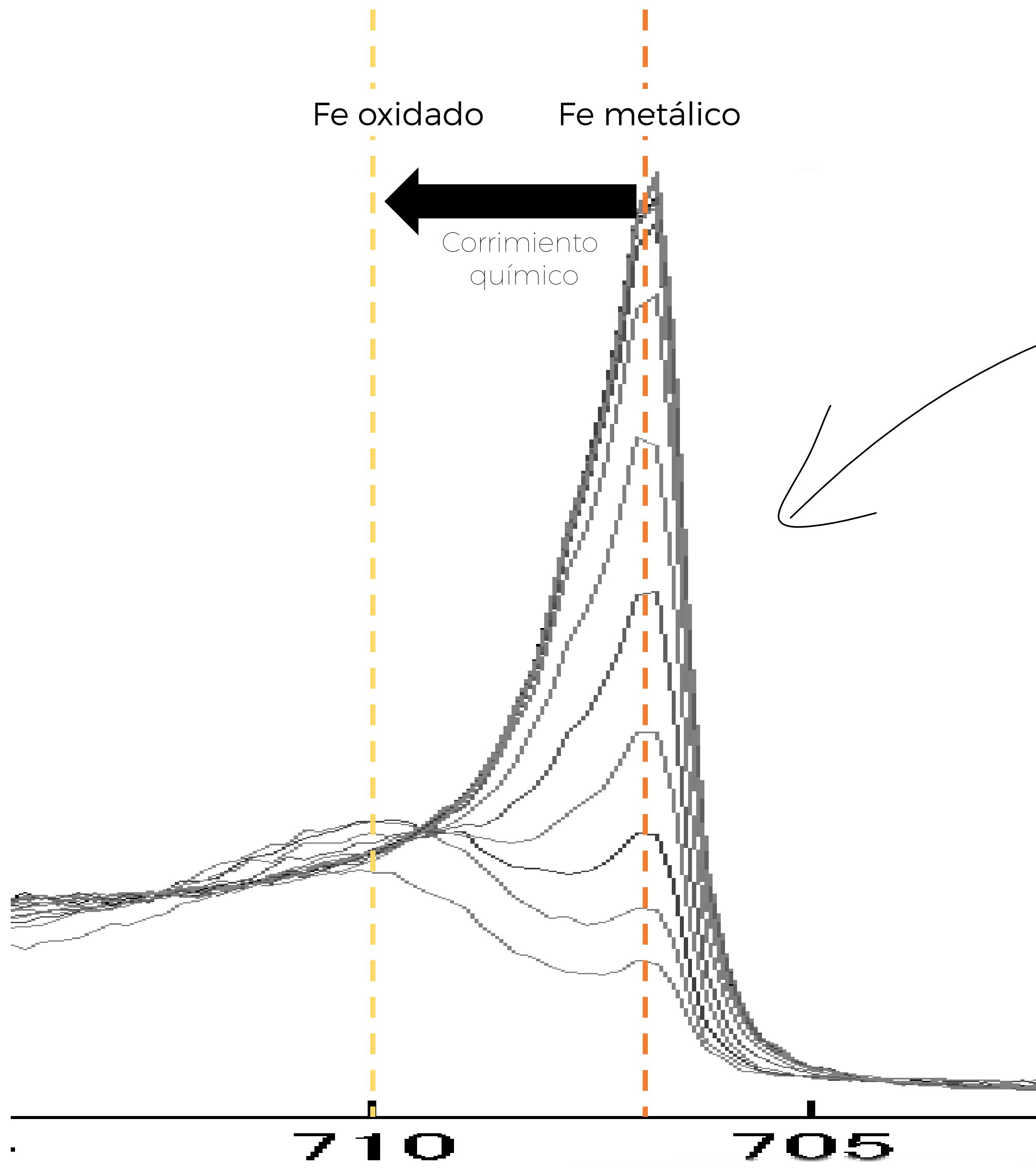


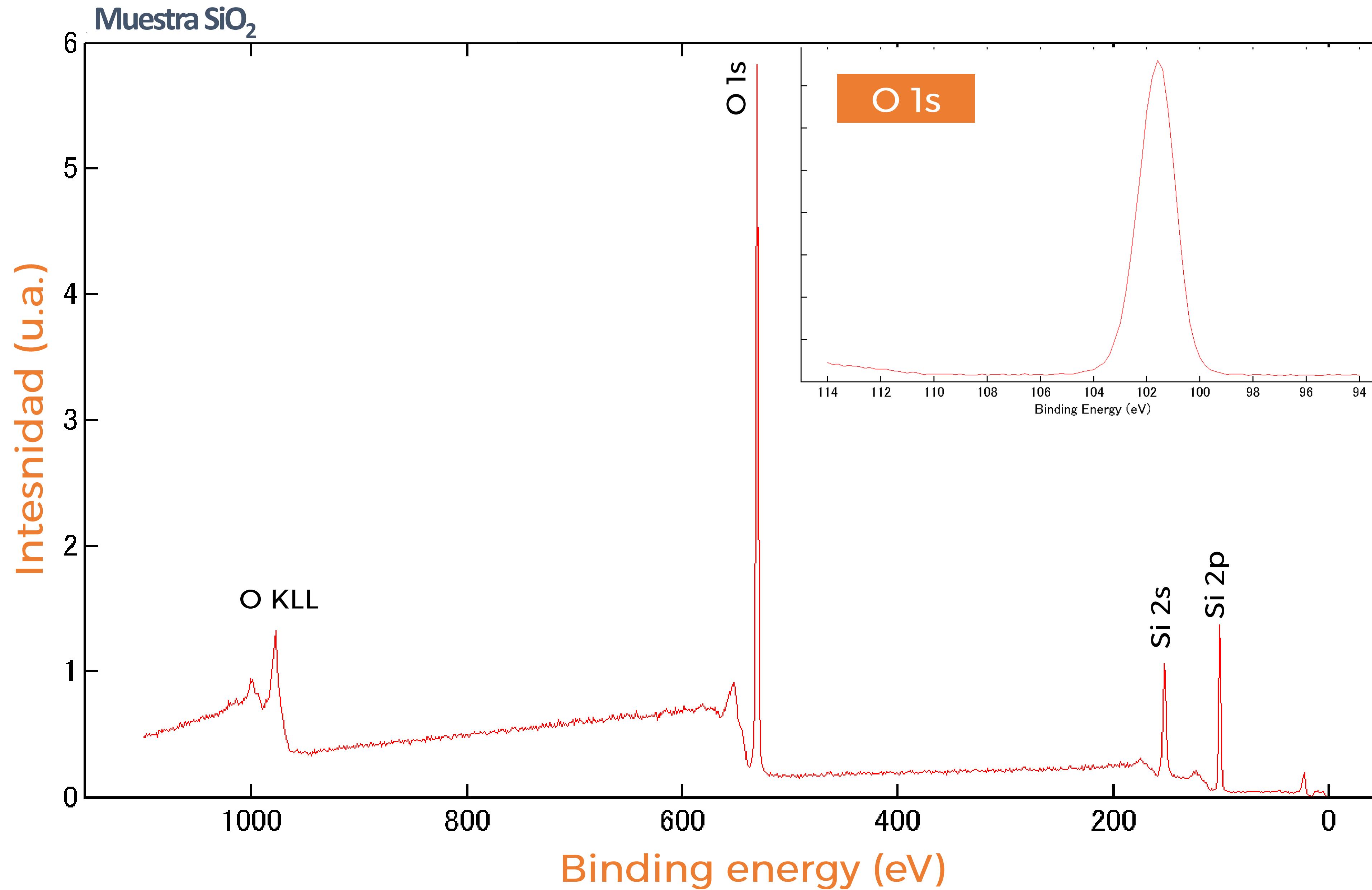


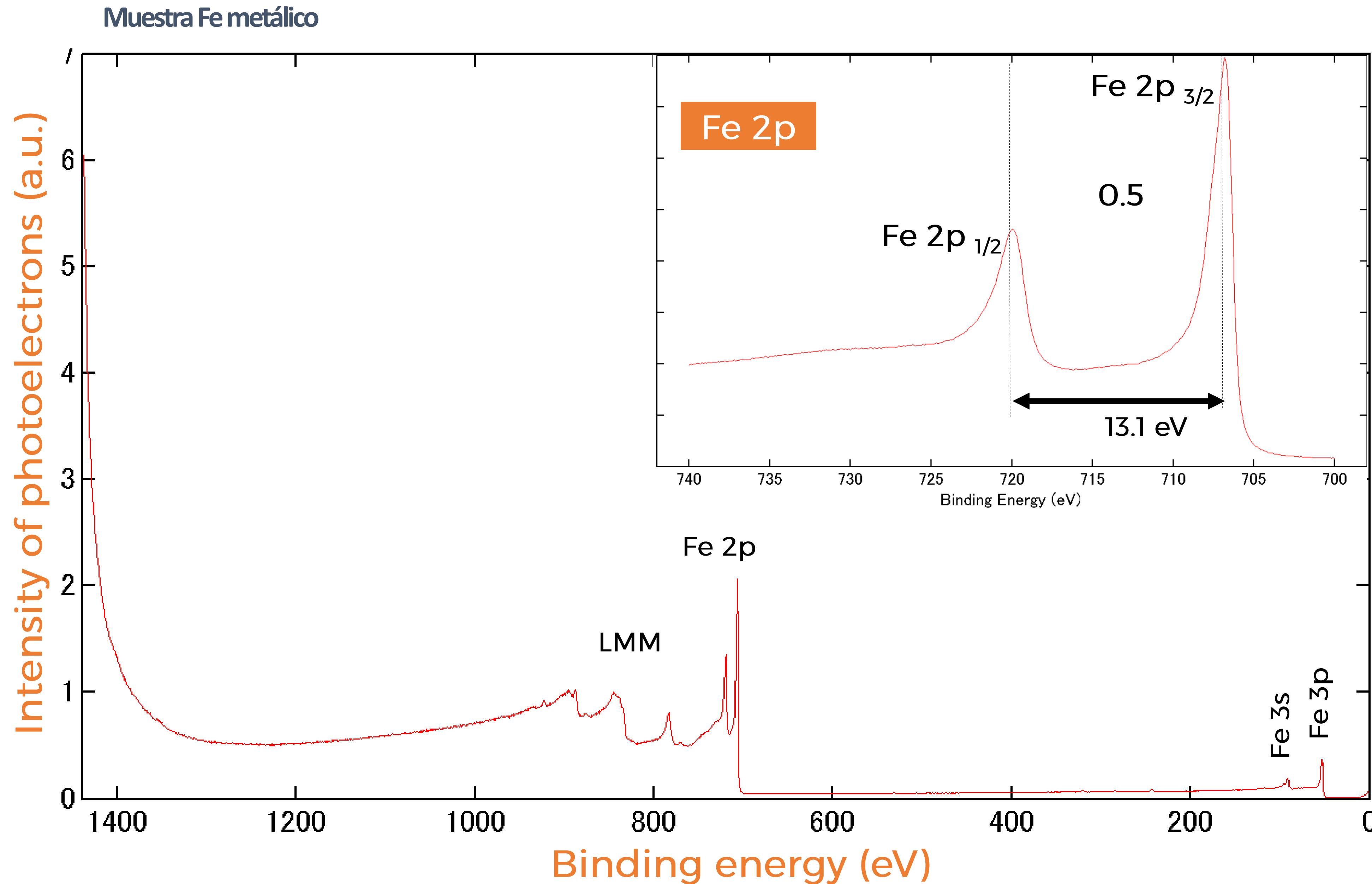


Los orbitales atómicos de la banda de valencia **interactúan** para generar nuevos orbitales moleculares. El efecto del **corrimiento** químico observado en los espectros de XPS es el **cambio** en la energía de enlace de los electrones en los **niveles profundos** de un elemento debido al cambio en el enlace químico

ESPECTROS Y SOFTWARE



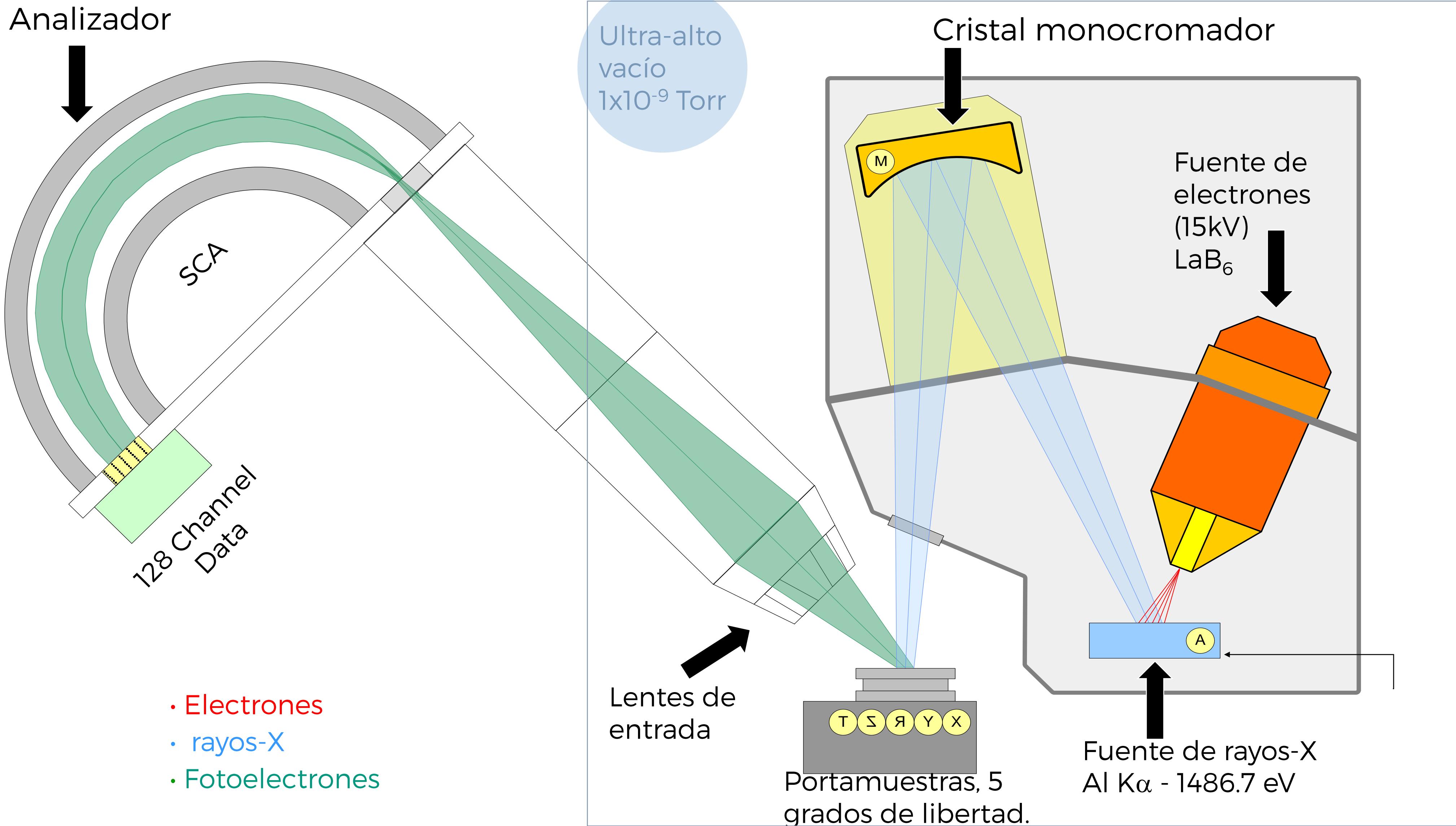




COMPONENTES BÁSICAS

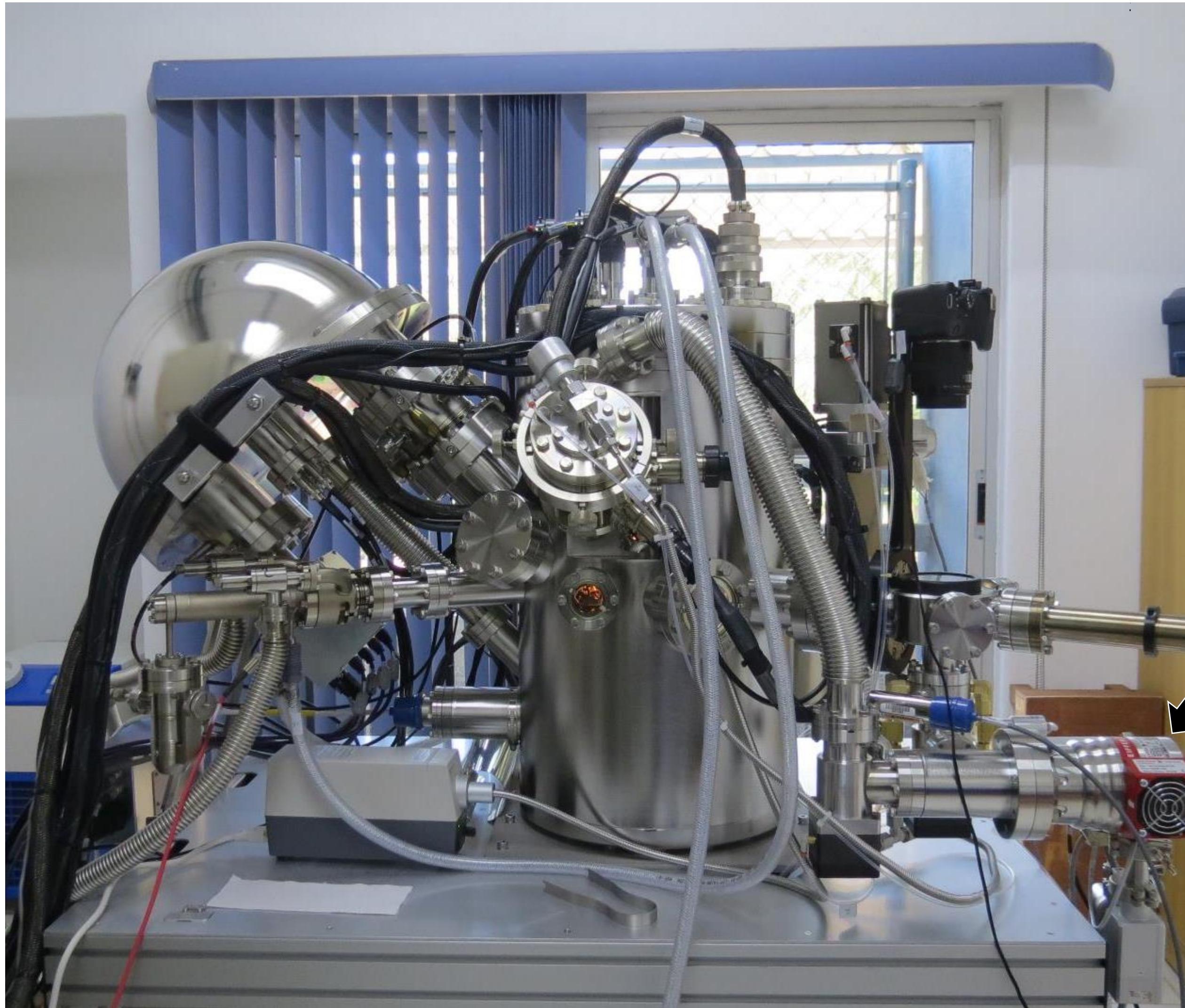


COMPONENTES BÁSICAS



COMPONENTES BÁSICAS

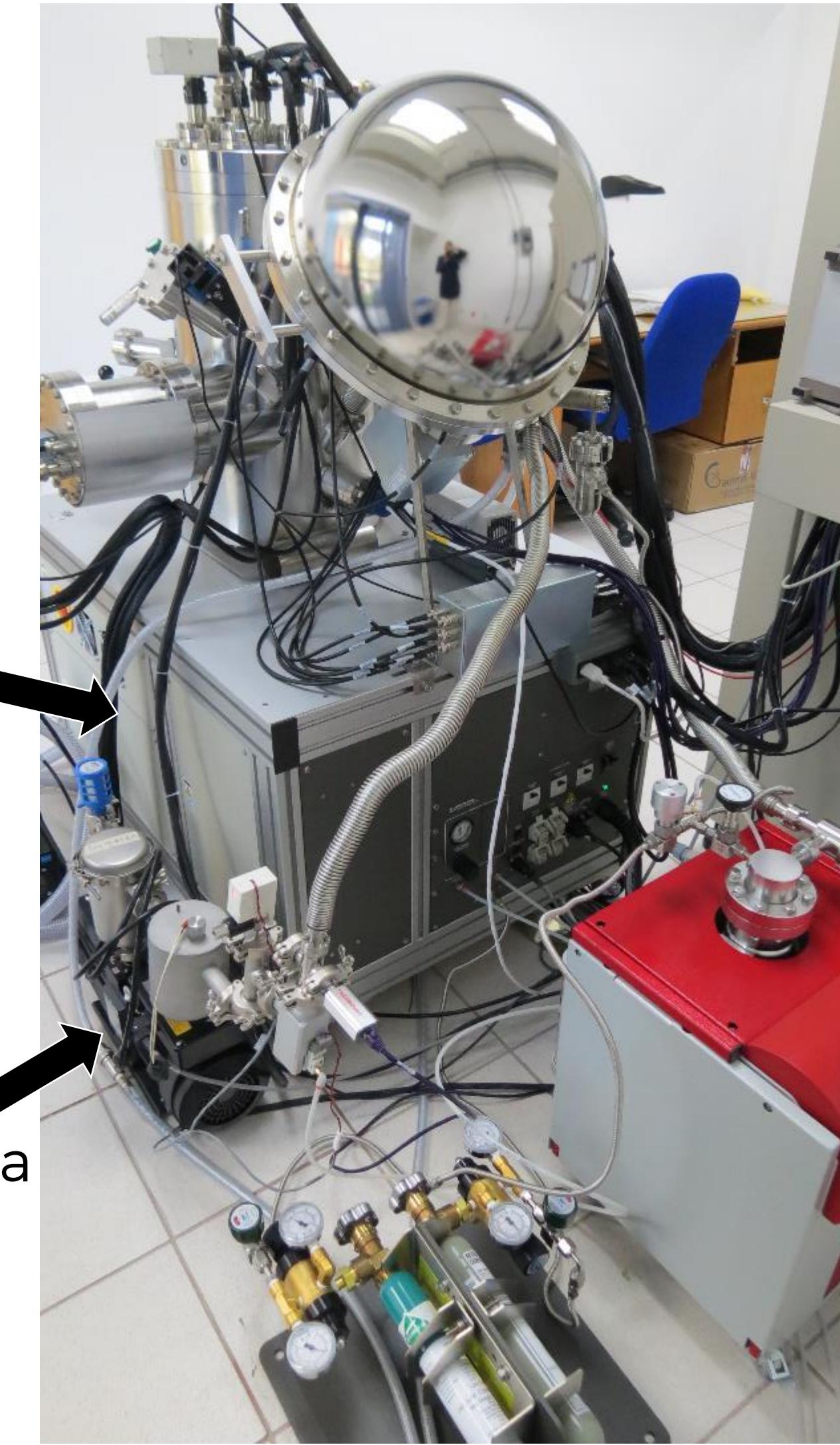
COMPONENTE DE VACÍO



Bomba
iónica

Bomba
turbo

Bomba
mecánica



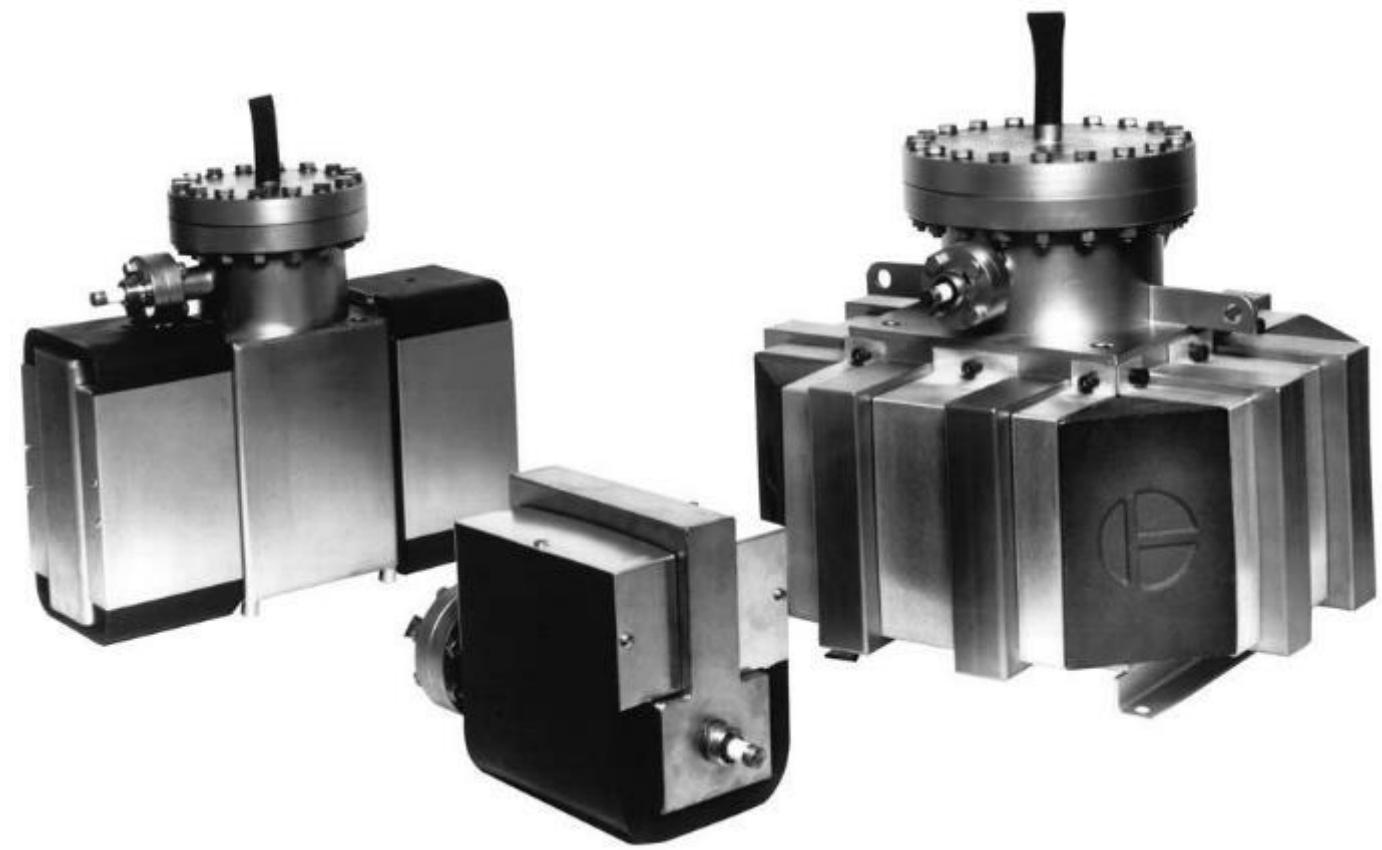
COMPONENTES BÁSICAS



Bomba mecánica
Ambiente- 1E-4 Torr



Turbomolecular
1E-4 Torr - 1E-8 Torr



Bomba iónica
1E-8 Torr - 1E-12 Torr



Sublimator ion pump
1E-6 Torr – 1E-12 Torr

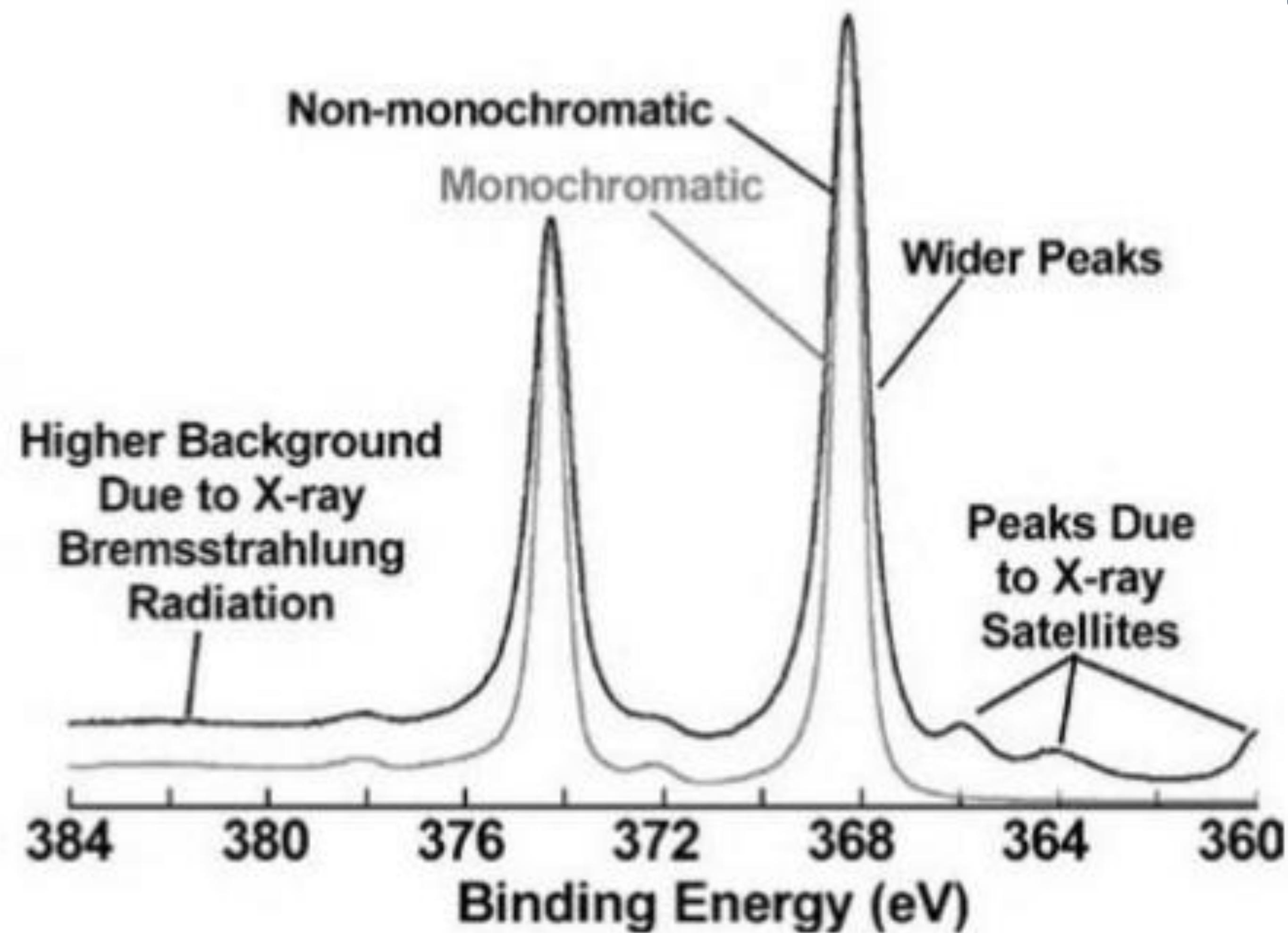
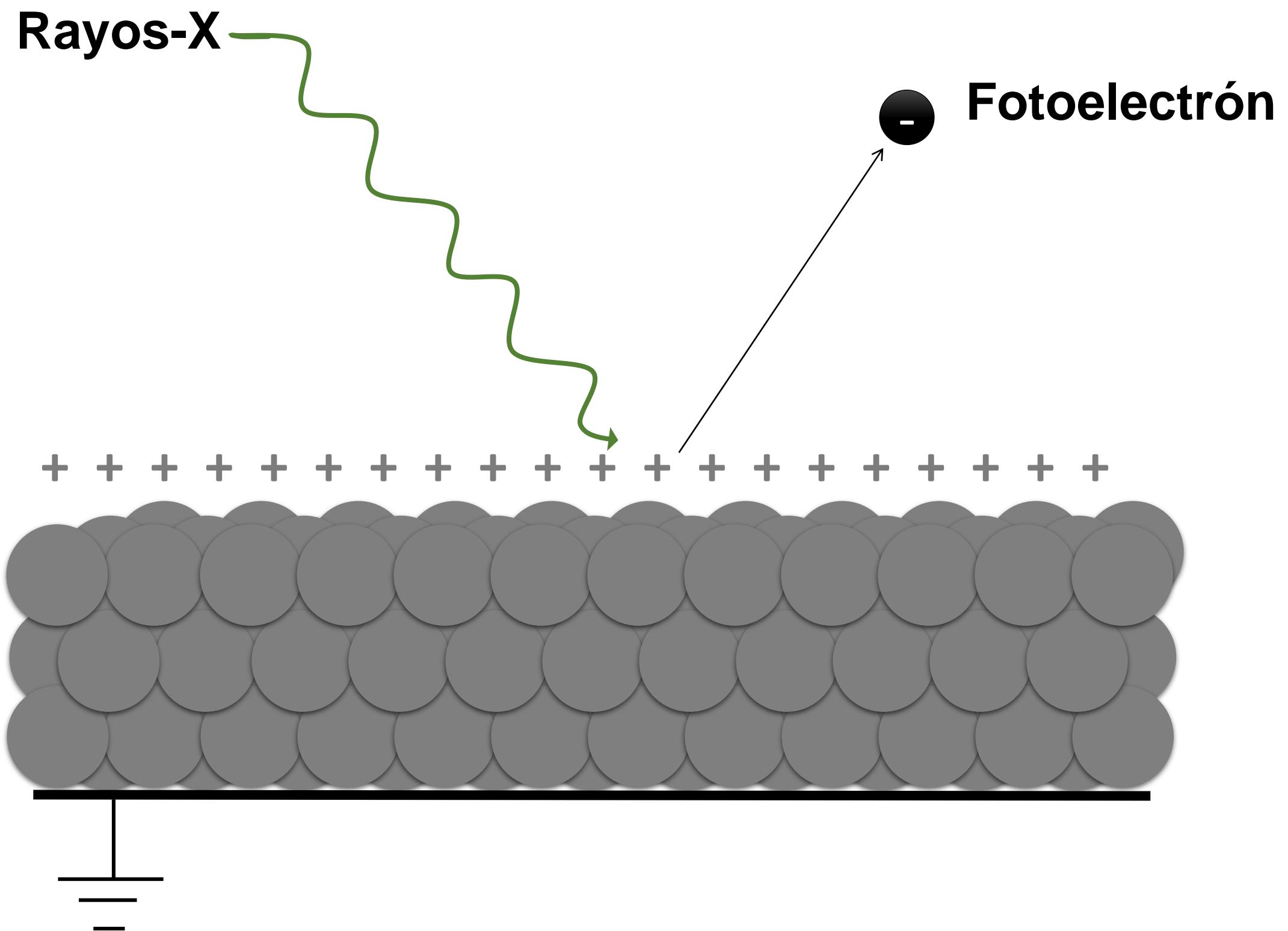
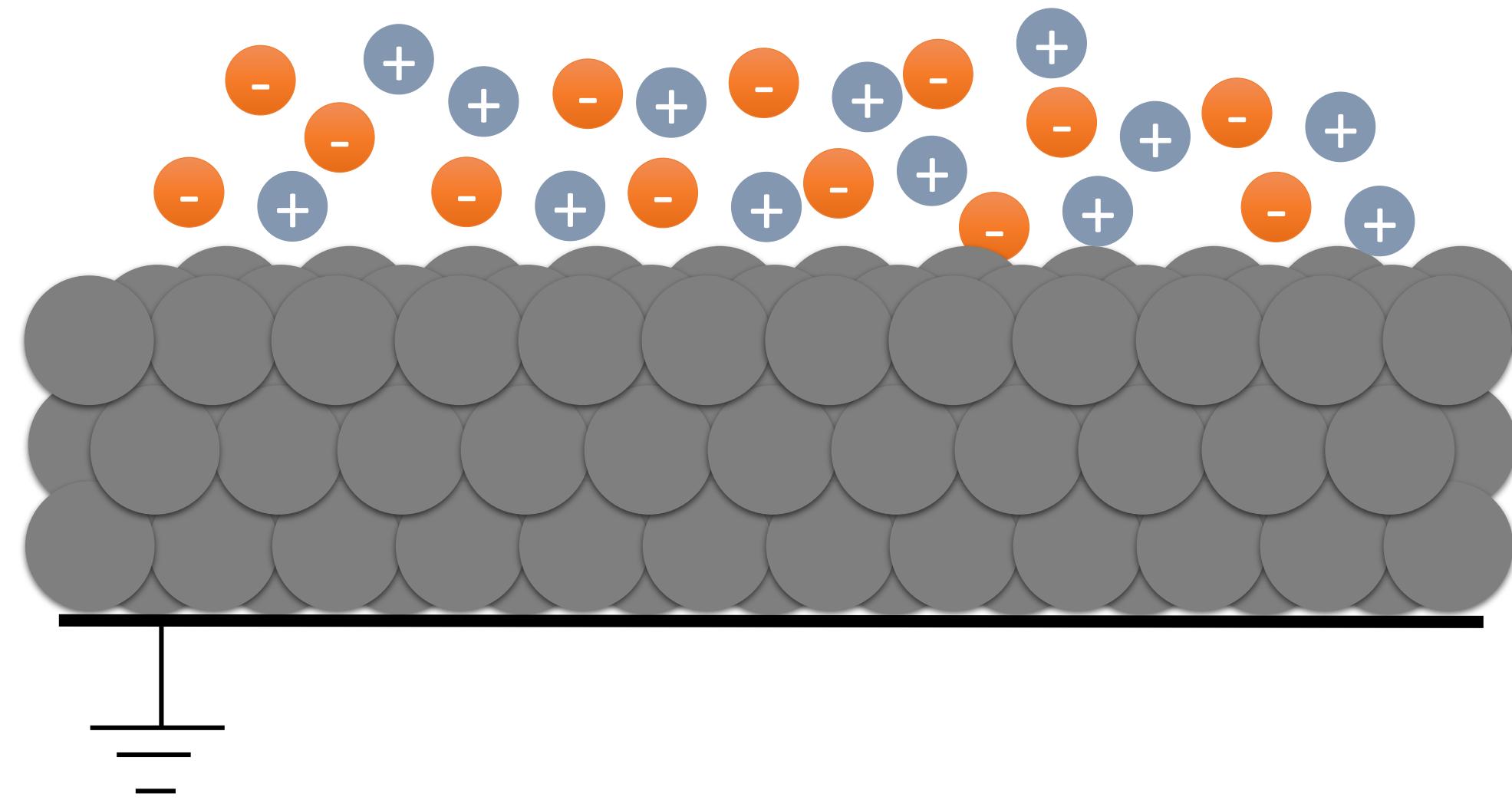


Figure 7 A comparison of the Ag 3d spectra acquired with monochromatic and nonmonochromatic X-rays. (The spectra are normalized to the maximum peak intensity.)

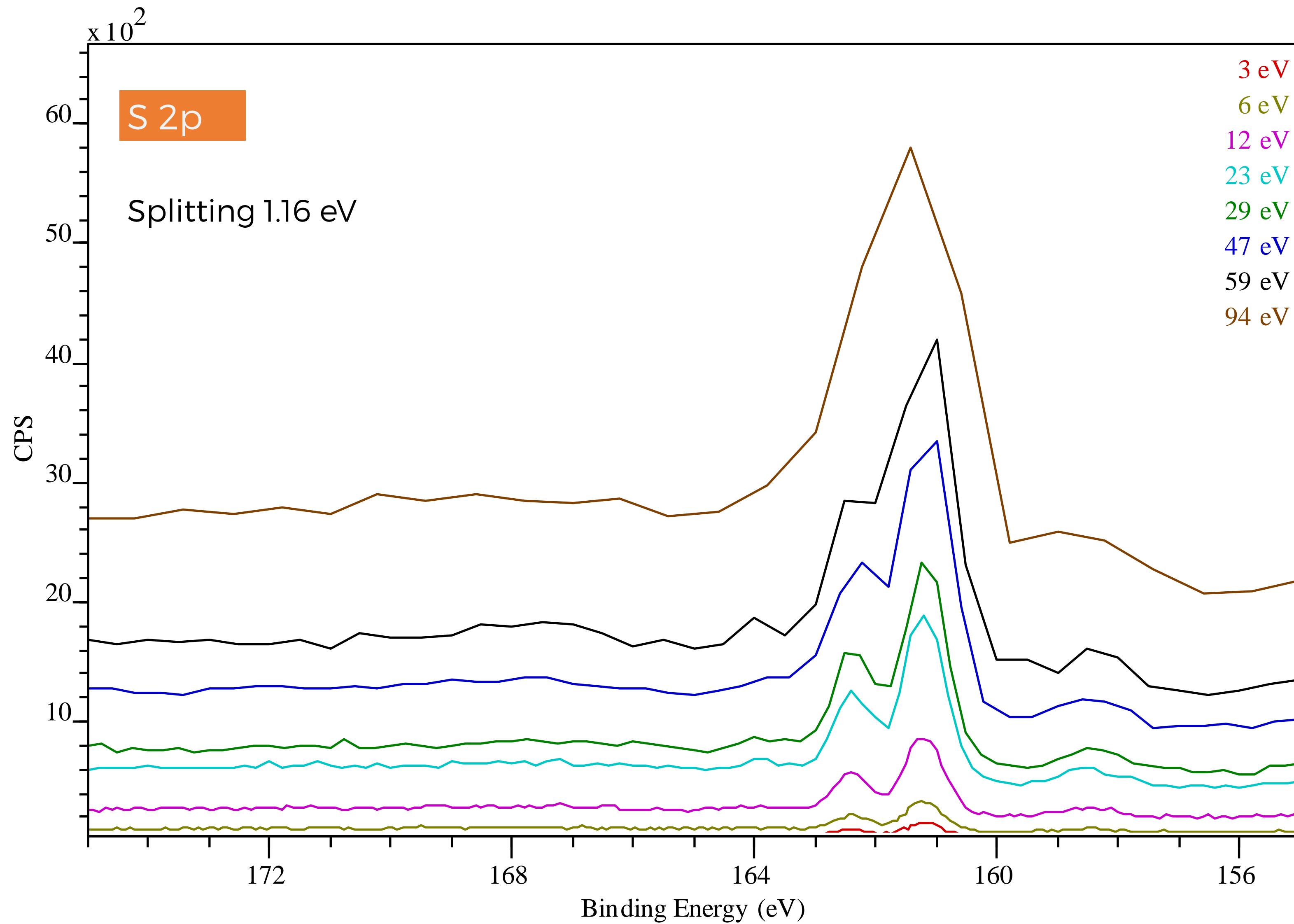


Ensanchamiento del pico y corrimiento
a altas energías de enlace



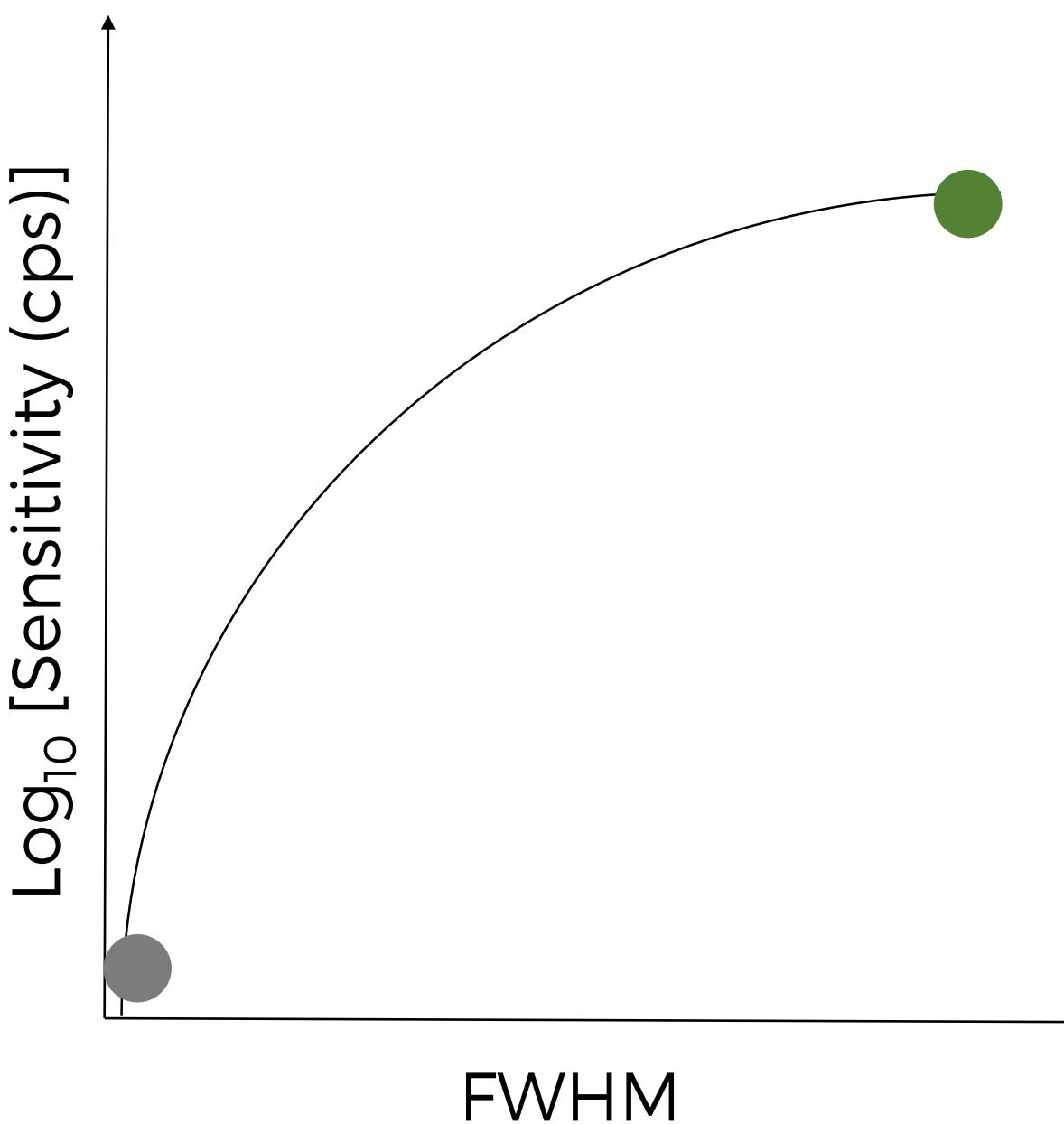
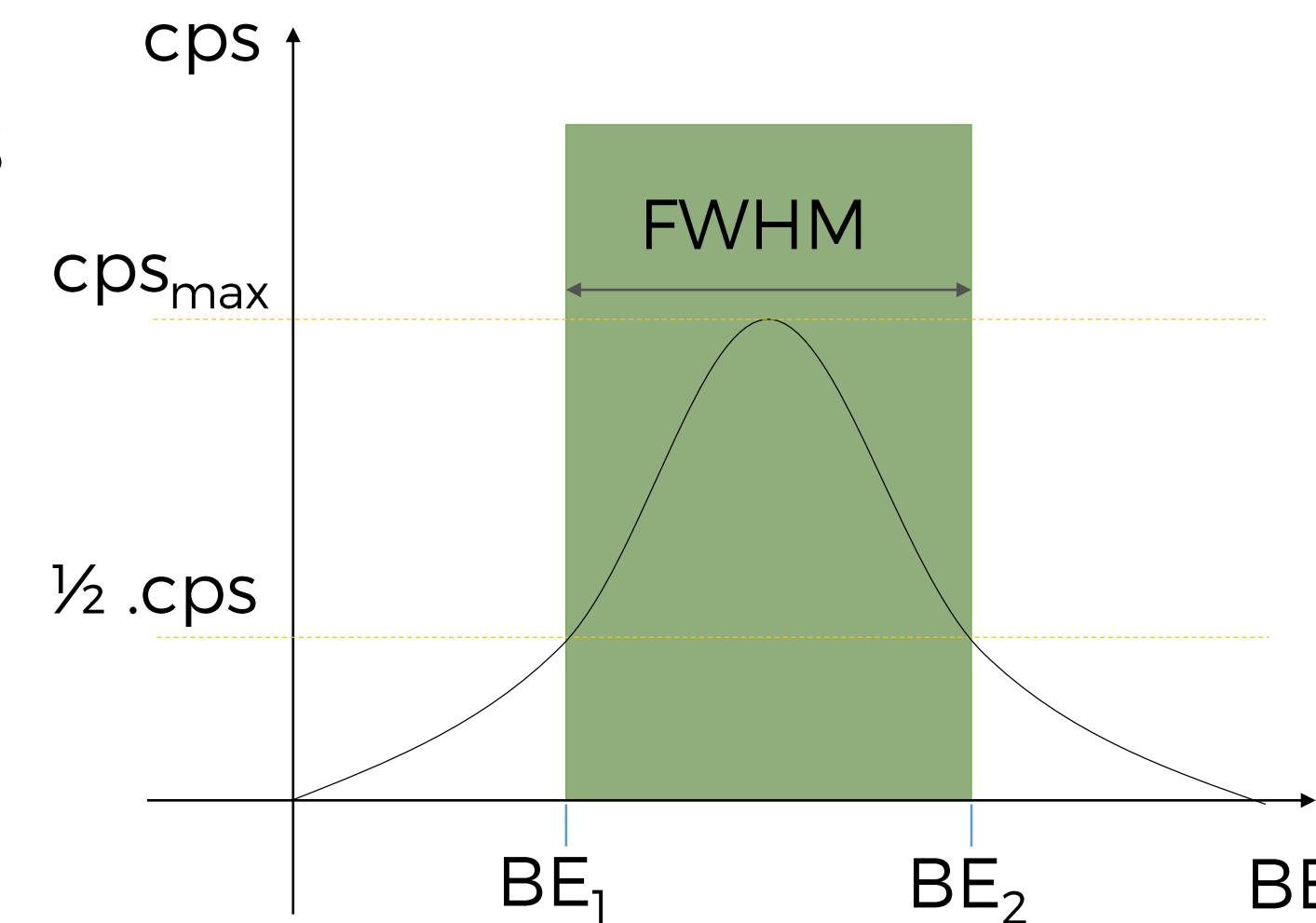
SISTEMA XPS

VARIACIÓN DE ENERGÍA DE PASO (ANALIZADOR)



SISTEMA XPS

- Full width half maximum (FWHM) es una medida de la resolución de XPS
 - Alto FWHM → baja resolución
 - Bajo FWHM → alta resolución
- Cuentas por Segundo (cps) es la cantidad de señal detectada
 - Altas cps → mayor sensitividad
 - Bajas cps → baja sensitividad



Use una energía de paso (pass energy) alta para baja concentración de elementos.

● max sensitivity, but lower resolution

Use baja energía de paso para obtener información de estados químicos

● lower sensitivity, but high resolution

BASES DE DATOS

ENERGÍAS DE ENLACE PARA ELEMENTOS Y ESPECIES QUÍMICAS COMUNES

1.0	Bi	6p1	3.9	Pt	5d	10.0	P	3p	18.0	At	6s	24.0	Kr	4s	34.0	K	3s	44.0	Ra	6s	52.0	Tm	5s	65.7	V	3s	
1.0	Ce	4f	4.0	Ir	5d	10.0	Ti	4s	18.0	Ce	5p	24.0	Sn	4d	35.0	Re	5p3	44.0	U	6s	52.3	Yb	5s	66.0	Ni	3p	
1.0	Co	3d	4.0	Pm	4f	10.0	V	4s	18.0	Pr	5p	25.0	Th	6p1	35.2	Mo	4p	44.4	Y	4s	52.6	Fe	3p	66.0	Pt	5p1	
1.0	Cr	3d	4.5	Ag	4d	10.0	Zr	5s	18.1	Hf	Ntv Ox		26.0	Bi	5d3	35.2	W	Na2WO4	45.0	Ta	5p1	53.0	Sn	loss	67.8	Ta	5s
1.0	Fe	3d	4.8	Dy	5d	10.5	Bi	6s	18.2	C	2s	26.0	He	1s	35.3	Y	loss	45.1	As	203	53.4	Os	4f5	68.0	Ra	5d	
1.0	Ga	4p	5.0	B	2p	10.7	Cd	4d5	18.4	Sr	4p	26.0	Rn	6s	35.8	W	O3	45.5	As	Ntv Ox	54.0	Os	5p1	68.0	Tc	4s	
1.0	Hf	5d	5.0	Br	4p	11.0	Kr	4p	18.7	Ga	3d5	26.1	Lu	5p	36.0	Ce	5s	45.7	Ge	loss	54.2	Se	CdSe	68.5	Br	3d5	
1.0	In	5p	5.0	Ca	3d	11.0	Rn	6p	18.8	Ga	3d	26.8	Ta	205	36.0	Gd	5s	46.0	Re	5p1	54.5	Se	GeSe	68.5	Br	KBr	
1.0	Na	3s	5.0	Er	4f	11.0	Sc	4s	18.9	Ga	3d3	26.8	Zr	4p	36.6	Sr	4s	46.3	Ga	loss	54.9	Se	3d5	68.8	Cd	4p	
1.0	Os	5d	5.0	Po	6p	11.1	Cs	5p3	19.0	Eu	5p	27.0	Br	4s	36.7	V	3p	46.8	Re	207	54.9	Li	1s	69.0	Br	3d	
1.0	Pb	6p	5.3	Se	4p	11.6	Cd	4d3	19.0	Nd	5p	28.2	Sc	3p	37.0	W	5p3	46.8	W	5p1	54.9	Li	OH	69.5	Br	3d3	
1.0	Sn	5p	5.5	Cl	3p	12.0	Cs	5p	19.0	Pb	5d5	28.6	In	loss	37.5	Hf	5p1	47.0	Mn	3p	54.9	Se	3d	70.0	Re	loss	
1.2	Yb	4f7	5.8	Au	5d	12.0	Po	6s	19.0	Ra	6p	28.8	Rb	4s	38.0	Pm	5s	47.0	Rh	4p	55.2	Se	GeSe2	71.0	Pt	4f7	
1.4	Pd	4d	6.0	Ta	5d	12.0	Te	5s	19.0	Sm	5p	29.0	Dy	5p1	38.0	Pr	5s	47.9	Ru	4p	55.3	Li	CO3	71.8	Mg	loss	
1.4	Rh	4d	6.0	Y	4d	12.0	Tl	5d5	19.1	Ga	Sb fract	29.0	Er	5p	38.3	Sn	loss	48.0	Dy	5s	55.6	Nb	4s	72.6	Pt	4f	
2.0	Cd	5p	6.2	Hg	5d	12.6	Cs	5p1	19.4	Ga	AlAs etch	29.0	Lu	5p	39.0	Eu	5s	48.0	Rn	5d	55.7	Se	3d3	72.7	Al	2p3	
2.0	Mg	3s	6.9	Eu	4f	13.0	Tl	5d	19.5	N	2s	29.1	Ge	3d5	39.0	Nd	5s	48.0	Sb	loss	56.8	Au	5p3	72.9	Al	2p	
2.0	Mo	4d	7.0	O	2p	13.2	Rb	4p	19.7	Ga	P fract	29.2	F	2s	39.0	Tc	4p	48.5	I	4d	56.8	Lu	5s	73.1	Tl	5p3	
2.0	Nb	4d	7.0	Sm	4f	13.2	Rb	4p	19.7	Ga	As fract	29.4	Ge	3d	39.5	Tm	5p	49.5	Ho	5s	57.4	Er	5s	73.2	Al	2p1	
2.0	Nd	4f	7.0	Sn	5s	14.0	Ne	2p	20.0	U	6p	29.5	Ho	5p1	40.0	At	5d	49.5	Mg	CO3	58.0	Ag	4p	73.8	Al	N	
2.0	Ni	3d	7.0	Xe	5p	14.0	Sc	3d	20.2	Zn	loss	29.7	Ge	3d3	40.0	Ba	5s	49.6	Mg	(OH)2	58.0	Fr	5d	74.0	Au	5p1	
2.0	Pr	4f	7.1	Lu	4f7	14.2	Hf	4f7	20.5	Gd	5p	30.2	Ge	Se	40.0	In	loss	49.6	Mg	2p3	58.0	Hg	5p3	74.2	Cr	3s	
2.0	Sb	5p	7.1	Tb	4f	15.0	Fr	6p	20.7	Ga	203	30.3	Na	2p	40.0	Tb	5s	49.7	Mg	O	58.1	W	loss	74.3	Al	203	
2.0	Sc	4p	7.7	Gd	4f	15.0	H	1s	21.0	Pb	5d3	30.9	Nb	4p	40.1	Te	4d	49.8	Mg	2p	58.2	Ti	3s	74.3	Al	203-nH2O	
2.0	Tc	4d	7.8	Dy	4f	15.0	Hf	4f	21.6	Ta	4f7	30.9	Pb	loss	40.2	Re	4f7	49.9	Mg	2p1	58.3	Te	loss	74.4	Pt	4f5	
2.0	Ti	3d	8.0	At	6p	15.0	Rb	4p1	21.8	Tb	5p	31.0	Hf	5p3	41.0	Ne	2s	50.0	Mg	CO3	58.6	Ag	4p	74.4	Al	(OH)3	
2.0	V	3d	8.0	S	3p	15.0	Tl	5d3	22.0	Dy	5p3	31.0	Po	5d	41.0	Sm	5s	50.0	Sr	loss	58.9	Y	loss	74.9	Cu	3p	
2.0	Yb	4f	8.3	Ho	4f	15.7	Cl	3s	22.0	Pm	5p	31.3	W	4f7	41.2	Re	4f	50.3	Zr	4s	59.0	Co	3p	74.9	Se	loss	
2.0	Zr	4d	8.3	Lu	5d	15.9	Hf	4f5	22.3	Ar	3s	31.5	Ge	Se2	41.4	Re	Ntv Ox		50.4	Mg	NtvOx1	59.2	As	loss	75.0	Cs	4d5
2.5	Yb	4f5	8.4	Lu	203	15.9	I	5s	22.7	Ta	4f	31.7	Sb	4d	41.5	As	3d5	50.7	Os	4f7	60.8	Ir	4f7	75.1	Pt	O2-nH2O	
2.6	Te	5p	8.5	Tm	4f7	16.0	K	3p	23.0	Cs	5s	32.1	Ga	loss	41.8	As	3d	50.7	Pd	4p	61.0	Mg	loss	75.1	W	5s	
2.8	Cu	3d	8.6	Lu	4f5	16.0	P	3s	23.1	O	2s	32.3	W	4f	42.0	As	S	50.7	Sc	3s	62.0	Ir	4f	75.5	Al	Ntv Ox	
2.8	Mn	3d	8.9	Ar	3p	16.0	S	3s	23.3	Ho	5p3	32.4	Ti	3p	42.0	Th	6s	50.9	Mg	reoxid	62.0	Ir	O2	76.0	Cs	4d	
2.8	Re	5d	9.0	F	2p	16.9	In	4d	23.3	Y	4p	32.6	Ta	5p3	42.1	Ca	3s	51.0	Ir	5p3	62.0	Ir	5p1	77.8	Ni	loss	
2.8	Si	3p	9.0	Ru	4d	17.0	La	5p	23.4	Ta	S2	33.0	La	5s	42.1	Cr	3p	51.0	Mg	NtvOx2	62.0	Mo	4s	78.3	In	4p	
2.8	W	5d	9.0	Sb	5s	17.0	Th	6p3	23.5	Ca	3p	33.2	Ge	O2	42.2	As	3d3	51.4	Os								

BASES DE DATOS

ENERGÍAS DE ENLACE PARA ELEMENTOS Y ESPECIES QUÍMICAS COMUNES

82.0	Br	loss	101.8	Si	Almand.	119.4	Ga	loss	137.8	Pb	203	158.9	Y	2(CO ₃) ₃	181.0	Ge	3s	204.1	Nb	NbO	235.3	Mg	Auger
82.0	Mn	3s	101.9	Hg	4f	119.4	Tl	CO ₃	137.8	Se	Auger	159.2	Bi	Ntv Ox	181.1	Zr	3d3	205.0	Nb	3d3	237.0	Pm	4p3
82.7	Pb	5p3	102.0	Pt	5s	120.0	Hg	5s	138.3	Pb	4f	159.6	Ho	4d5	181.2	Br	3p3	205.1	S	loss	237.6	Ta	4d3
84.0	Au	4f7	102.0	Si	3N4	120.0	Tl	4f	138.5	Ge	loss	160.0	Bi	5s	182.0	Br	3p	205.8	Lu	4d3	237.9	Rb	3p3
84.0	Ba	4d3	102.6	Si	O	121.0	Pm	4d	138.8	Pb	Ntv Ox	161.2	S	PbS	182.0	Fr	5p1	206.1	Nb	NbO ₂	238.0	Cs	4s
84.7	Ba	4d	102.9	Zn	loss	121.1	I	4p	139.0	Pb	CO ₃	161.3	Ho	203	182.1	Yb	4d5	207.0	Ce	4p3	238.0	Rn	4f
85.0	Au	4f	103.0	Ga	3p	122.0	Ge	3p3	139.0	Xe	4p	161.5	S	Cu ₃ , TaS ₂	182.4	Zr	O2	207.0	Xe	4s	238.9	Mo	loss
85.0	Th	5d5	103.0	Ga	3p3	122.1	Tl	4f5	139.5	Zn	3s	161.7	Se	3p3	182.8	Er	Auger	207.3	P	loss	241.8	Ar	2p3
86.0	Ba	4d5	103.0	Pt	loss	122.4	Cu	3s	140.0	Fr	5p3	161.9	S	HgS	183.7	Si	loss	207.4	Nb	Nb ₂ O ₅	242.0	Ar	2p
86.9	Kr	3d5	103.0	Si	O2	122.4	In	4s	140.3	Gd	4d5	162.2	S	MoS ₂	184.0	Po	4f	207.4	Nb	Ntv Ox	243.1	W	4d5
87.2	Kr	3d	103.0	U	5d3	127.0	Rn	5p3	140.7	As	3p3	162.3	Bi	4f5	184.9	Yb	203	208.0	Kr	3p3	243.9	Ar	2p1
87.7	Au	4f5	103.5	Si	O ₂ -nH ₂ O	128.2	Eu	4d5	141.2	Gd	203	162.4	S	Na ₂ S ₂ O ₃	185.3	S	loss	210.0	At	4f	245.0	Nd	4p1
88.0	Al	loss	103.7	Al	loss	128.3	Tl	loss	141.7	Pb	4f5	162.6	S	FeS ₂	185.5	I	4s	210.8	Hf	4d5	248.0	Ba	4s
88.1	Au	2O ₃	103.9	Hg	4f5	128.6	P	InP etch	142.0	As	3p	163.9	S	2p3	187.8	Br	3p1	210.9	Dy	Auger	248.0	Rb	3p1
88.2	Kr	3d3	104.0	La	4d	129.0	Ge	3p1	145.9	Tb	4d5	164.0	Rn	5p1	187.9	B	CrB	213.0	B	loss	249.6	S	loss
88.2	Pd	4s	104.0	Po	5p3	129.0	P	InP etch	146.0	Sr	loss	164.0	S	2p	188.0	B	1s	213.0	La	4p1	250.0	Sm	4p3
88.3	Zn	3p	106.3	Pb	5p1	129.0	Sm	4d	147.0	As	3p1	164.0	Sr	loss	188.0	B	MoB, LaB ₆	214.0	Rn	5s	253.0	Mo	loss
89.0	Os	5s	107.0	Ga	3p1	129.3	P	GaP etch	148.0	At	5p1	165.1	S	2p1	188.1	B	WB	217.5	Cl	loss	253.0	Tc	3d
89.1	Mg	2s	108.0	Au	5s	130.0	Be	loss	148.0	Pb	5s	166.6	S	Na ₂ SO ₃	188.2	B	Ni3B	218.0	Pr	4p3	253.0	Tc	3d5
90.6	Sn	4p	109.7	Rb	3d5	130.0	Ho	Auger	148.5	Tb	F3	167.3	Er	4d5	188.9	B	Ntv Ox	220.5	Se	Auger	254.0	Ra	5s
91.0	Fe	3s	109.7	Rb	OAc	130.1	P	2p3	148.8	Al	loss	167.3	Se	3p1	189.0	P	2s	221.3	Hf	4d3	255.0	Br	3s
92.8	Bi	5p3	109.9	Cd	4s	130.6	P	2p	149.8	Pb	loss	167.6	Si	loss	189.2	Tm	Auger	223.0	Ce	4p1	255.0	Eu	4p3
93.0	Th	5d3	110.0	Ce	4d	131.4	P	2p1	149.9	P	loss	168.5	Er	203	190.8	B	N	225.7	As	3s	255.0	Pm	4p1
94.0	U	5d5	110.0	Rb	3d	132.0	Po	5p1	149.9	Tb	3O ₇	168.5	S	Na ₂ SO ₄	190.9	Yb	4d3	226.1	Ta	4d5	255.1	Se	Auger
94.6	Tl	5p1	110.5	Ni	3s	132.7	Ga	loss	150.5	Si	2s	168.5	S	Na ₂ S ₂ O ₃	194.0	B	2O ₃	228.0	Mo	3d5	255.6	W	4d3
95.2	Ir	5s	110.6	Mg	loss	133.4	Al	loss	152.0	Zn	loss	168.6	P	loss	195.0	At	5s	228.0	Nd	4p3	257.0	Tc	3d3
96.0	Br	loss	111.2	Rb	3d3	133.6	Si	loss	152.3	Dy	4d5	168.8	Y	loss	195.0	U	5p3	229.0	S	2s	260.0	Re	4d5
97.0	Ag	4s	111.8	Be	1s	133.7	Sr	3d5	152.9	Sb	4s	169.1	Te	4s	196.0	Lu	4d5	229.4	Mo	O ₂ (?)	260.0	U	5p1
98.7	Er	Auger	112.6	Te	4p	133.7	Sr	CO ₃	153.0	Ra	5p3	169.3	Er	4d3	196.1	Zr	loss	229.5	Mo	3d	261.0	As	Auger
99.8	Si	2p3	113.6	Be	O	134.0	Sr	3d	155.8	Y	3d5	173.0	Ba	4p	197.0	La	4p3	229.7	Mo	S ₂	261.5	Tb	Auger
99.8	Mg	loss	114.7	Be	Ntv Ox	134.9	Sm	2O ₃	156.1	Dy	2O ₃	173.3	Ga	loss	197.5	Ge	Auger	229.9	Se	3s	264.3	Rb	loss
99.9	Hg	4f7	115.0	At	5p3	135.5	Sr	3d3	156.6	Y	2O ₃	175.4	Tm	4d	198.4	Se	Auger	230.0	As	Auger	267.5	S	loss
100.1	Si	2p	115.0	Pr	4d	135.6	Eu	2O ₃	157.0	Bi	4f7	175.9	Tb	loss	198.7	Cl	2p	231.1	Mo	3d3	267.7	W	loss
100.2	Si	O	115.5	Se	Auger	136.8	Pb	O ₂	157.0	Bi	4f	176.3	Tm	2O ₃	198.9	Cl	2p3	232.6	Mo	Ntv Ox	268.0	Fr	4f
100.4	Si	2p1	116.2	Si	loss	136.8	Rb	loss	157.0	Bi	loss	177.0	Po	5s	198.9	Cl	MCl	232.9	Tb	Auger	268.4	Sr	3p3
100.4	Si	C	117.7	Tl	4f7	136.9	Pb	4f7	157.0	Y	3d	177.0	Th	5p3	199.8	Cl	C-Cl	233.0	Kr	3p1	270.0	Cl	2s
100.6	Sb	4p	117.9	Al	2s	137.0	Tl	5s	157.9	Y	3d3	178.7	Se	Auger	200.0	Ra	5p1	233.1	Mo	O ₃	271.3	Gd	4p3
100.7	Hg	O	118.0	Nd	4d</																		

BASES DE DATOS

ENERGÍAS DE ENLACE PARA ELEMENTOS Y ESPECIES QUÍMICAS COMUNES

278.7	Sr	3p1	301.6	Mg	Auger	340.3	Pd	3d3	382.0	U	4f	412.7	Lu	4p1	460.2	Gd	Auger	515.0	Eu	Auger	560.0	Pd	3p1
279.0	Os	4d5	305.0	Pr	4s	341.4	Ge	Auger	384.9	Tl	4d5	420.4	Ta	loss	462.5	Ta	4p1	515.6	V	2p	560.9	Ti	2s
280.1	Ru	3d5	305.5	K	loss	342.0	Th	4f5	386.0	Tm	4p1	421.6	Mo	loss	463.1	In	loss	515.9	V	203	562.8	Ta	4s
281.0	Ru	Ntv Ox	307.2	Rh	3d5	343.0	Ho	4p1	388.0	U	4f5	423.3	W	4p3	464.0	Bi	4d3	517.1	V	205	565.0	Na	Auger
281.1	Ru	O2	308.5	Rh	Ntv Ox	343.0	Zr	3p1	388.3	Se	Auger	424.5	N	loss	466.1	Ru	3p3	517.3	V	O2	567.0	Rn	4d3
282.2	Ru	3d	308.9	Rh	203	346.5	Pd	loss	389.8	K	loss	425.0	As	Auger	466.8	Nb	3s	518.5	Re	4p1	568.1	Cu	Auger
282.6	C	VC	308.9	Sr	loss	346.6	Ca	2p	390.3	Yb	4p1	425.0	Tc	3p3	468.0	As	Auger	519.0	As	Auger	570.9	Ga	Auger
282.9	C	NbC	309.4	Rh	3d	347.1	Ca	O	391.7	Ga	Auger	425.5	Pb	loss	468.5	Tm	4s	519.6	Pt	4p3	572.5	Te	CdTe
283.0	C	TaC	310.4	Ge	Auger	347.2	Mg	Auger	391.7	Mg	Auger	429.6	Zr	3s	471.0	Os	4p3	519.7	V	2p1	572.9	Te	3d5
283.0	Sm	4p1	311.0	Tb	4p1	347.8	Ca	UHV Ox	393.8	Mo	3p3	433.0	Ge	Auger	471.5	Zn	Auger	521.3	Rh	3p1	573.0	Zn	Auger
284.0	Tb	Auger	311.1	Y	3p1	349.0	Sm	4s	393.8	Y	3s	434.3	Pb	4d3	473.0	Po	4d5	524.0	Na	Auger	573.6	Ag	3p3
284.2	Ru	3d3	311.9	Ir	4d3	353.0	Au	4d3	395.6	Tb	4s	436.0	Ho	4s	474.0	Se	Auger	524.8	Ge	Auger	574.1	Cr	B
284.5	C	HOPG	311.9	Rh	3d3	357.2	Sr	3s	397.0	N	CrN	437.3	Hf	4p1	474.7	In	loss	528.2	Sb	3d5	574.3	Cr	2p3
284.5	Se	Auger	312.5	Mg	Auger	357.9	Ge	Auger	397.1	N	AlN	437.8	Ca	2s	480.8	Yb	4s	529.4	O	Ag2O, NiO	575.0	Cr	2p
285.0	C	1s	313.0	C	loss	357.9	Mg	Auger	397.3	N	TiN	440.0	Bi	4d5	484.9	Sn	3d5	529.6	Sb	203	575.5	Cr	Ntv Ox
285.4	C	C-OR	314.5	Pt	4d5	358.3	Hg	4d5	397.6	N	Si3N4	443.6	Ge	Auger	486.3	Sn	O	529.8	O	MgO	575.6	Cr	2O3
286.0	Cl	loss	315.1	Se	Auger	358.6	Se	Auger	398.4	N	1s	443.8	In	3d5	486.4	Ga	Auger	530.5	O	NaOH	576.5	Te	O2
286.0	Tb	4p3	315.2	Ho	4p3	359.0	As	Auger	398.4	N	BN	444.3	In	203	487.3	Sn	O2	531.1	O	Al2O3	576.6	Cr	Ntv Ox
287.0	C	C-Cl	319.5	Ar	2s	359.2	Lu	4p3	398.4	Sc	2p3	444.4	In	Ntv Ox	488.4	Ru	3p1	531.1	Sb	205	577.0	Fr	4d5
287.8	C	C=O, C-F	320.0	Nd	4s	359.3	Zr	loss	399.8	Se	Auger	444.8	In	P fract	488.8	Ho	Auger	531.8	O	1s LiOH	577.0	Te	3d
288.9	C	COOR	320.8	Er	4p3	360.8	Nb	3p3	399.9	Tm	Auger	444.9	In	GaAs	490.5	W	4p1	532.3	Pd	3p3	577.2	Hg	4p3
289.0	Eu	4p1	321.2	K	loss	363.0	Eu	4s	400.6	Ta	4p3	445.0	Tc	3p1	493.3	Sn	3d3	532.5	Ga	Auger	577.7	Cr	Ntv Ox
289.0	Kr	3s	321.8	Rb	3s	363.6	Ga	Auger	401.0	Sc	2p	445.2	In	Ntv OH	494.6	Zn	Auger	532.5	O	B2O3, SiO2	578.2	Ir	4p1
289.4	C	MCO3	322.0	U	5s	363.7	Dy	Auger	401.9	Sc	203	445.9	In	Ntv CO3	494.8	Ir	4p3	532.6	Sb	3d	579.5	Cr	O3
290.0	Ce	4s	323.6	Mg	Auger	366.0	Er	4p1	402.2	N	H4	446.4	Re	4p3	496.3	Rh	3p3	532.9	O	HgO	579.8	Ge	Auger
290.6	Gd	4p1	326.8	Ge	Auger	366.8	Ag	2s	403.2	Sc	2p1	446.9	Pb	loss	497.1	Se	Auger	533.0	At	4d3	580.0	Cr	KCrO4
290.8	C	C-CO3, CF2	329.4	Zr	3p3	367.7	Ag	O	404.1	Cd	O	447.3	Ga	Auger	497.2	Sn	3d	533.8	Hf	4s	581.8	Zn	Auger
291.7	C	pi->pi*	331.0	Pm	4s	368.2	Ag	Ag, Ag2O	405.0	Cd	3d5	448.0	In	3d	497.4	Na	Auger	536.4	Na	Auger	583.3	Te	3d3
292.7	C	CF3	331.2	Pt	4d3	368.5	Mg	Auger	405.1	Cd	Te	450.3	Er	4s	498.0	Sc	2s	537.6	Sb	3d3	583.5	Cr	2p1
292.9	K	2p3 KX	332.0	Dy	4p1	370.0	Eu	Auger	405.4	Cd	Se, CO3	451.4	In	3d3	499.0	Sn	loss	541.0	Rn	4d5	586.2	Er	Auger
293.0	Os	4d3	332.3	Tm	4p3	371.0	Ag	3d	405.5	Tl	4d3	453.0	Se	Auger	500.0	Po	4d3	544.0	Tc	3s	586.9	Tm	Auger
294.0	Th	5s	333.0	Th	4f7	371.0	As	Auger	406.7	Cd	(OH)2	453.9	Ti	2p3	503.8	Ga	Auger	544.2	Sb	loss	588.9	Ga	Auger
295.0	K	2p	333.1	Mg	Auger	374.2	Ag	3d3	407.2	N	O3	454.3	Na	Auger	505.0	Mo	3s	546.3	Au	4p3	591.0	Ru	3s
295.6	Dy	4p3	334.0	Au	4d5	376.0	Gd	4s	408.0	Cd	3d	455.1	Ti	O	507.0	At	4d5	548.0	Os	4p1	593.6	W	4s
295.7	K	2p1	335.0	Pd	3d5	376.2	Nb	3p1	411.0	Tb	Auger	456.0	Ti	2p	507.5	Sn	loss	548.1	Cu	Auger	600.0	Gd	Auger
296.2	Ir	4d5	335.4	Pd	Ntv Ox	377.2	K	2s	411.3	Mo	3p1	457.4	Ti	203	507.9	Lu	4s	552.4	Na	Auger	600.7	Te	loss
296.2	Se	Auger	337.0	Pd	O	377.3	U	4f7	411.7	Cd	3d3	458.0	As	Auger	512.1	V	2p3	553.2	O	loss	603.0	Fr	4d3
299.0	Ra	4f	337.5	Pd	3d	377.8	Hg	4d3	412.0	Pb	4d5	458.2	Ti	CaTiO3	513.2	Na	Auger	553.3	Sb	loss	603.0	Ra	4d5
299.2	Y	3p3																					

BASES DE DATOS

609.6	Tl	4p3	675.0	Xe	3d	724.0	Pt	4s	819.7	Te	3p3	915.9	Cr	Auger	999.0	O	Auger	1107.0	N	Auger	1243.8	Pd	Auger
617.0	Cd	3p3	676.0	Th	4d5	724.8	Cs	3d5	826.0	In	3s	918.6	Cs	Auger	1003.0	Nd	3d3	1108.0	Sm	3d3	1245.9	Tl	Auger
619.0	I	3d	676.7	In	loss	724.8	Cs	Cl	830.5	Co	Auger	925.3	Co	2s	1003.6	Cr	Auger	1109.8	Cd	Auger	1249.0	Ge	2p1
619.2	I	3d5	677.9	Tm	Auger	724.9	Cs	2O-SiO2	833.0	Ce	Auger	929.0	Rn	4p1	1004.8	Te	3s	1112.9	Sb	Auger	1250.8	Pt	Auger
619.2	I	KI	679.0	Bi	4p3	736.0	U	4d5	833.0	F	Auger	930.9	I	3p1	1008.7	Ni	2s	1116.6	Ga	2p3	1259.8	Ru	a
623.2	Ni	Auger	680.2	Hg	4p1	740.0	At	4p3	835.2	La	2O3	931.7	Cu	Cl	1013.0	O	Auger	1117.7	Sc	Auger	1264.2	Mo	Auger
625.2	Re	4s	682.0	Sm	Auger	740.0	Cs	3d3	836.0	La	3d5	931.8	Pr	3d5	1014.7	V	Auger	1126.0	Eu	3d5	1265.0	Rh	Auger
626.1	Ho	Auger	682.4	Xe	3d3	748.0	Ho	Auger	836.5	Te	loss	932.0	Cs	Auger	1020.3	Te	Auger	1128.0	La	3p3	1265.8	Ge	loss
626.4	V	2s	685.1	F	CaF2	749.0	Cs	loss	837.2	La	B6	932.3	Cu	S	1021.7	Zn	O	1128.9	Ag	Auger	1272.0	Ce	3p1
627.8	Rh	3s	685.7	F	1s	756.2	Sn	3p1	837.9	Co	Auger	932.4	Cu	2O	1021.8	Zn	2p3	1129.0	Sn	Auger	1272.0	U	4p1
628.2	Cu	Auger	685.7	F	LiF	758.0	Nd	Auger	841.1	Gd	Auger	932.6	Cu	2p3	1022.3	Zn	S	1131.8	Te	Auger	1275.7	Tb	3d3
629.4	Ga	Auger	688.9	F	CF2	761.1	Pb	4p1	844.2	Cs	Auger	932.9	Cu	2O	1022.5	Sb	Auger	1135.0	Ag	Auger	1296.2	Dy	3d5
630.6	I	3d3	690.9	Ir	4s	761.2	Au	4s	846.0	Fe	Auger	933.9	Cu	O	1027.0	Pm	3d5	1137.0	Ba	3p1	1298.6	Mo	Auger
634.5	Er	Auger	695.7	Cr	2s	761.8	Cs	loss	846.7	Tl	4s	934.0	Xe	3p3	1027.2	Cr	Auger	1141.0	Xe	3s	1303.3	Mg	1s
635.0	Cu	Auger	697.4	Co	Auger	763.4	Gd	Auger	851.0	Po	4p1	934.6	Cu	(OH)2	1031.0	Zn	loss	1143.4	Ga	2p1	1304.0	Cl	Auger
636.0	Ra	4d3	700.3	Tb	Auger	766.4	Sb	3p3	851.6	Mn	Auger	936.6	Bi	4s	1031.9	Sb	Auger	1148.9	Sc	Auger	1307.0	Hf	Auger
638.7	Mn	2p3	702.0	Ne	Auger	768.0	Rn	4p3	852.6	Ni	2p3	940.7	Cu	CT	1034.9	Tl	Auger	1151.0	In	Auger	1315.3	Mg	loss
640.4	Ni	Auger	703.1	In	3p1	768.6	Mn	2s	852.9	Ni	B	942.2	Cu	CT	1042.0	At	4s	1153.0	Fr	4s	1316.1	Pt	Auger
640.5	Ga	Auger	703.5	F	loss	770.2	Sn	loss	853.0	La	3d3	943.8	Cu	CT	1043.0	U	4p3	1155.0	Eu	3d3	1318.0	Ta	Auger
640.9	Mn	Mn3O4	705.0	Po	4p3	772.8	Cd	3s	853.8	Ni	O	944.0	Sb	3s	1044.8	Zn	2p1	1159.4	Pd	Auger	1319.0	Nb	Auger
641.0	Mn	MnO	705.2	Ni	Auger	777.7	Ni	Auger	854.3	Ni	Ntv Ox	944.1	Mn	Auger	1049.6	Sn	Auger	1170.0	Th	4p1	1321.6	Lu	Auger
641.0	Mn	Mn2O3	706.7	Fe	2p3	778.3	Co	2p3	855.4	Ni	(OH)2	945.5	Sb	Auger	1052.0	Pm	3d3	1184.0	Ce	3p3	1322.3	Re	Auger
641.6	Mn	MnO2	707.2	Fe	S2	779.0	U	4d3	859.0	F	Auger	952.2	Cu	2p1	1055.3	V	Auger	1185.5	Rh	Auger	1323.9	As	2p3
642.4	Au	4p1	707.5	Ga	Auger	779.2	Co	O	863.0	Ne	1s	952.2	Pr	3d3	1055.5	Zn	loss	1186.8	Gd	2O3	1324.5	Mo	Auger
643.5	I	loss	709.8	Fe	O	779.5	Co	3O4	869.9	Ni	2p1	952.5	Cs	Auger	1058.0	Ra	4p1	1186.9	Gd	3d5	1326.3	Mg	loss
643.6	Pb	4p3	710.4	Fe	2O3-g	780.0	Ba	3d5	870.5	Cs	Auger	959.5	Cr	Auger	1058.0	Sn	Auger	1190.0	Ag	Auger	1334.0	Pt	Auger
645.0	Mn	2p	710.5	Fe	3O4	780.0	Ba	CO3, OAc	870.7	Te	3p1	959.9	Te	Auger	1063.0	Ba	3p3	1194.0	Ca	Auger	1335.1	Dy	3d3
647.5	Cu	Auger	710.8	Fe	2O3-a	780.6	Co	(OH)2	875.0	I	3p3	965.0	Th	4p3	1067.7	Tl	Auger	1196.4	Zn	2s	1337.7	Zr	Auger
649.7	Mn	2p1	711.5	Fe	OOH	780.9	Co	Ntv Ox	878.1	F	Auger	969.3	Te	Auger	1071.8	Na	2O-SiO2	1208.0	Ra	4s	1352.9	Ho	3d5
651.0	Cd	3p1	711.6	F	loss	782.2	Sb	loss	879.0	Ra	4p3	970.4	I	Auger	1071.9	Na	OH	1213.0	Pd	Auger	1358.7	Er	3d5
652.2	Zn	Auger	712.2	Ni	Auger	784.0	Fe	Auger	882.0	Ce	O2	976.8	V	Auger	1072.0	I	3s	1217.0	Cs	3s	1359.5	As	2p1
655.0	Eu	Auger	713.0	Co	Auger	793.7	Co	2p1	884.0	Ce	3d5	979.7	O	Auger	1072.0	Na	1s	1217.0	Ge	2p3	1363.6	Yb	Auger
655.7	Ga	Auger	713.0	Th	4d3	795.2	Ba	3d3	885.2	Sn	3s	980.0	Fr	4p1	1072.0	Na	Cl	1217.0	Ru	Auger	1365.5	Mo	Auger
657.2	I	loss	714.1	In	loss	797.0	Pr	Auger	886.0	At	4p1	981.0	Nd	3d5	1076.4	In	Auger	1219.6	Gd	3d3	1367.1	Tm	Auger
658.0	Os	4s	714.6	Sn	3p3	802.0	Ba	loss	886.5	Ba	Auger	981.8	I	Auger	1081.0	Sm	3d5	1221.4	C	Auger	1368.2	Zr	Auger
659.4	Zn	Auger	715.1	Er	Auger	803.6	Hg	4s	888.0	Fe	Auger	994.6	Te	Auger	1084.0	In	Auger	1225.0	Ag	Auger	1373.3	Tb	3p3
665.2	In	3p3	719.5	Cu	Auger	805.0	Bi	4p1	888.4	Te	loss	995.0	Po	4s	1092.5	Te	Auger	1234.7	Rh	Auger	1378.9	Gd	3p3
665.3	Ho	Auger	719.6	Ag	3s	808.9	Tb	Auger	891.7	Pb	4s	995.0	Sb										

BASES DE DATOS



NIST XPS



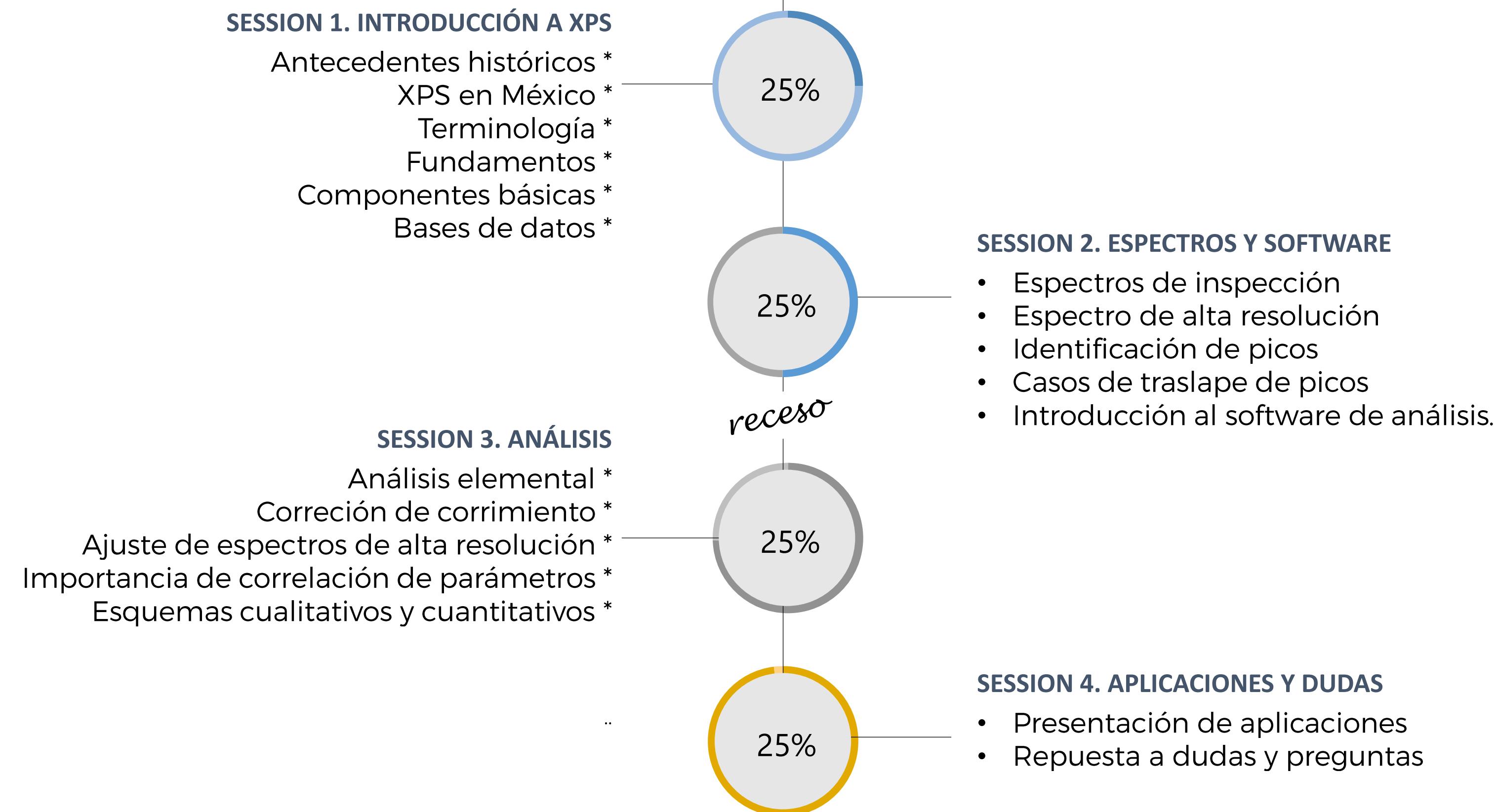
THERMO XPS

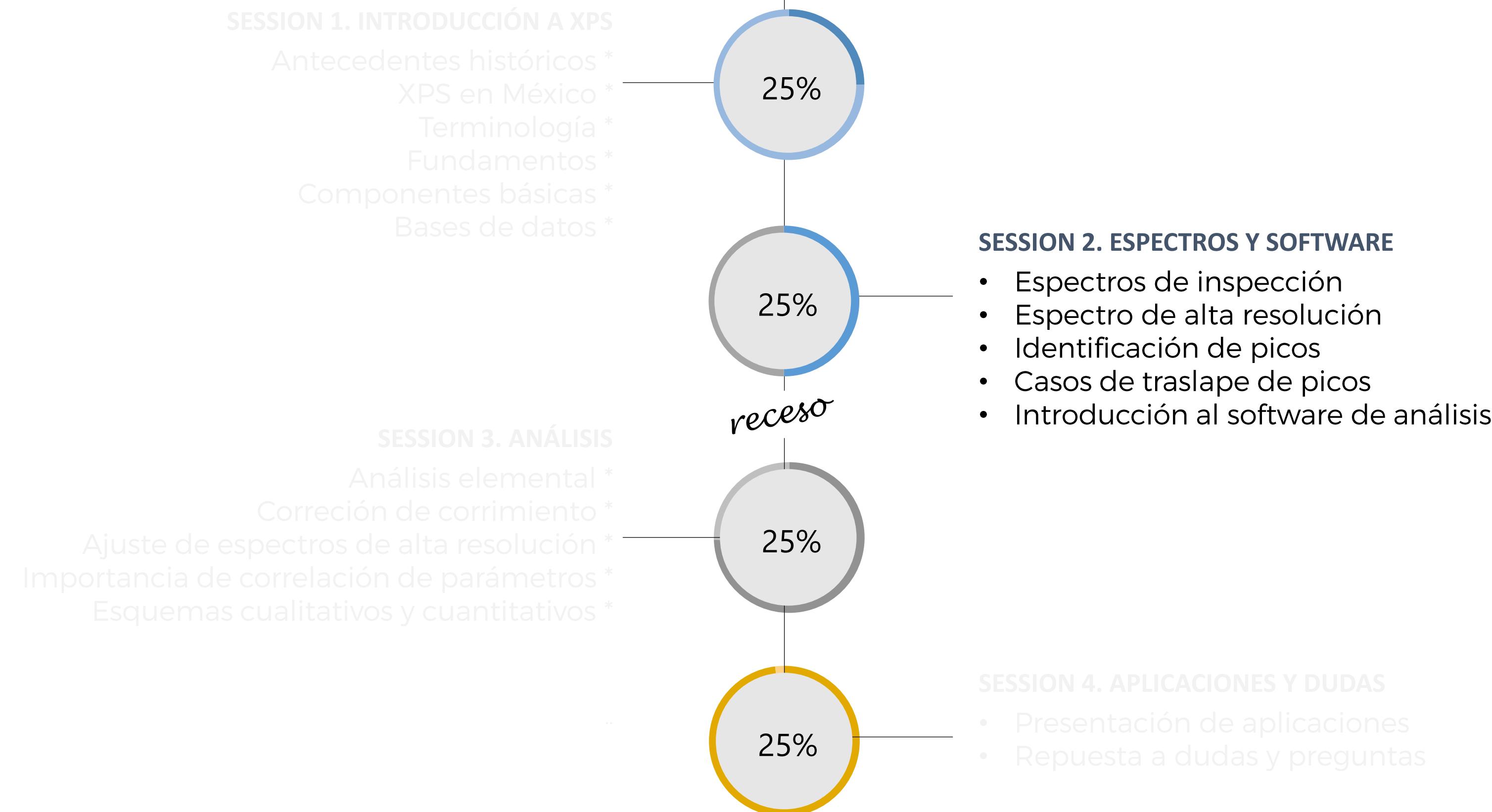


SURFACE SCIENCE
WESTERN XPS



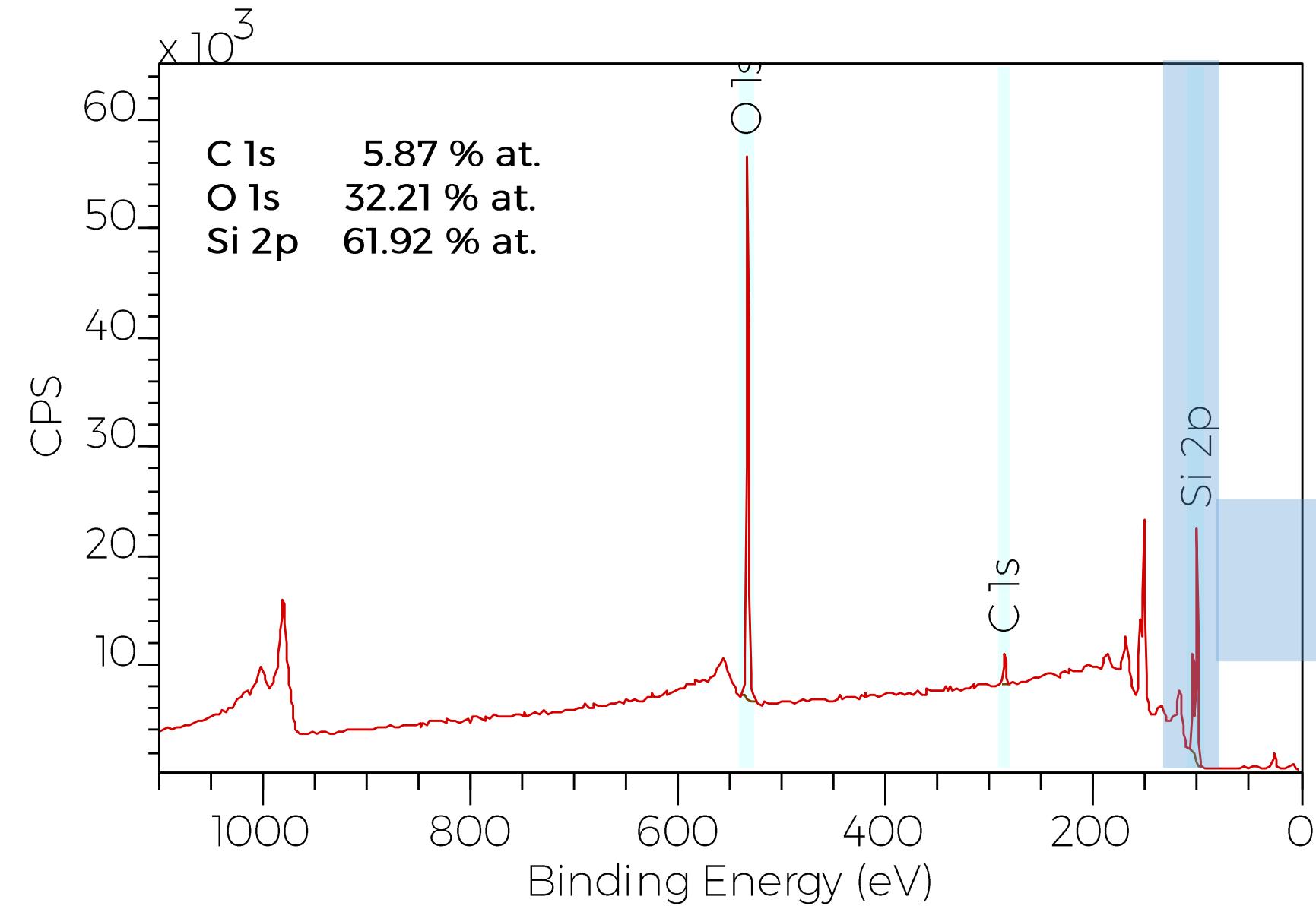
CROSS SECTIONS





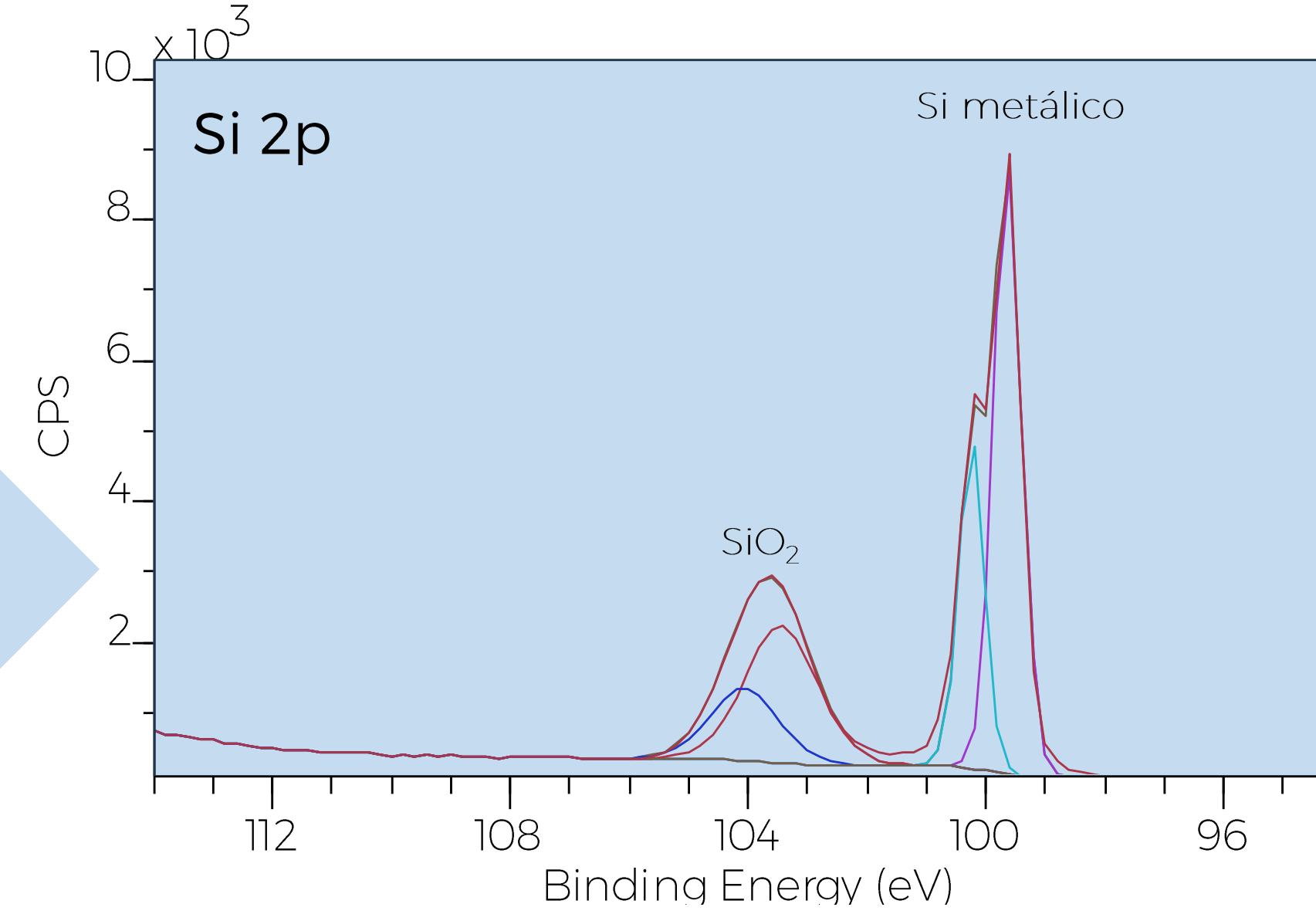
ESPECTROS Y SOFTWARE

ESPECTROS DE XPS



01 COMPOSICIÓN ELEMENTAL

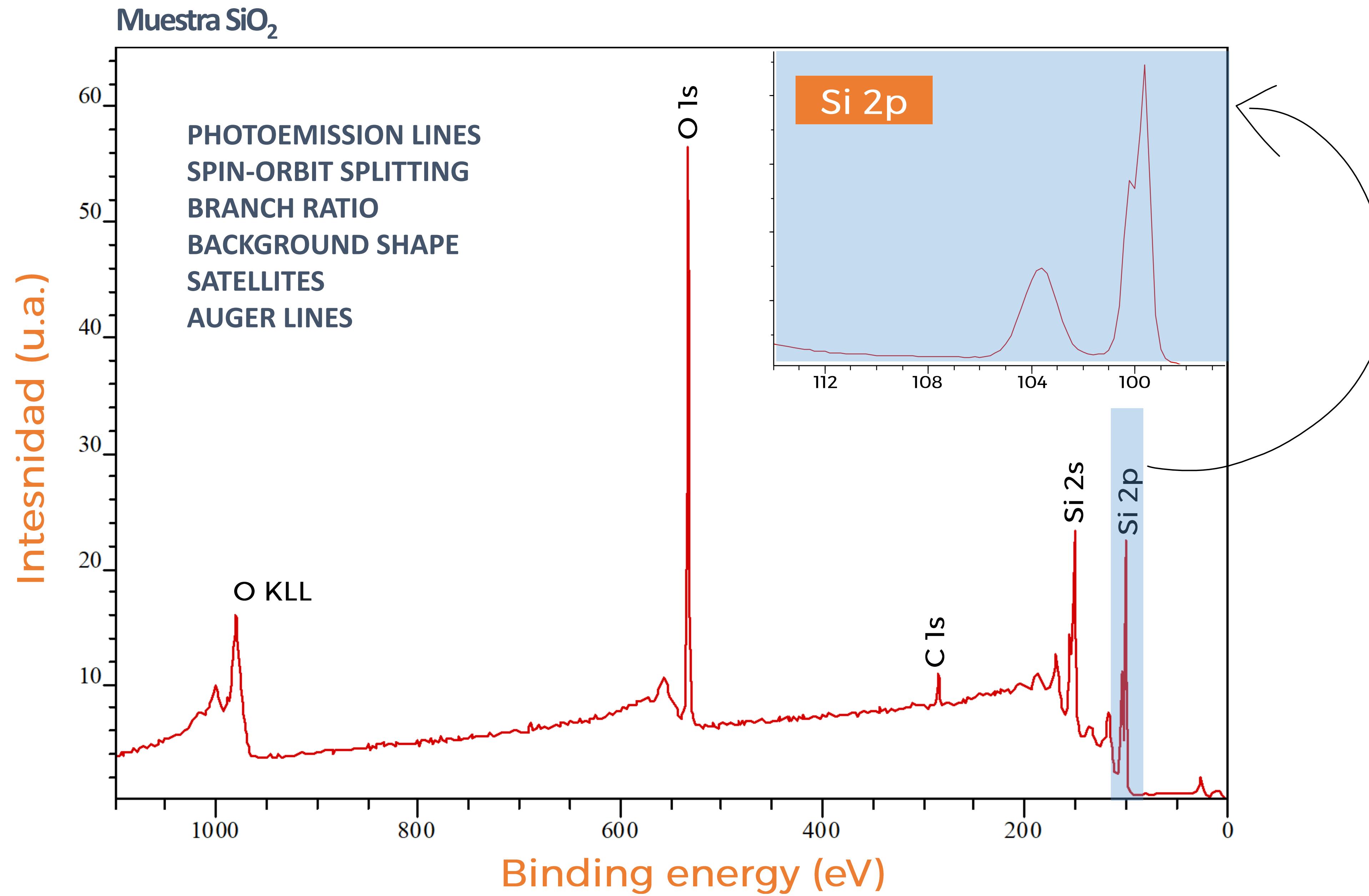
Identificación de elementos y determinación de su concentración en porcentajes atómicos (% at.)



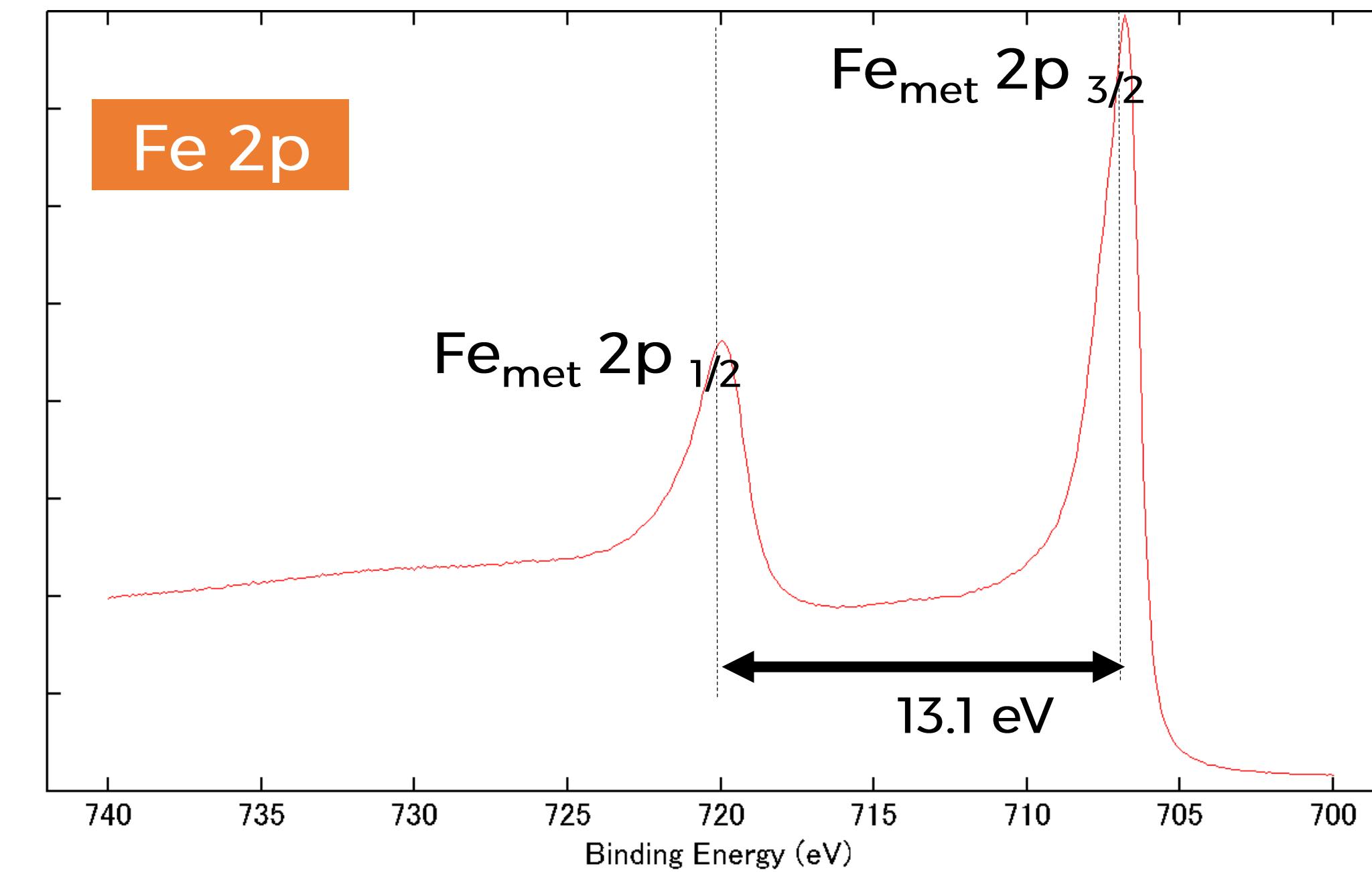
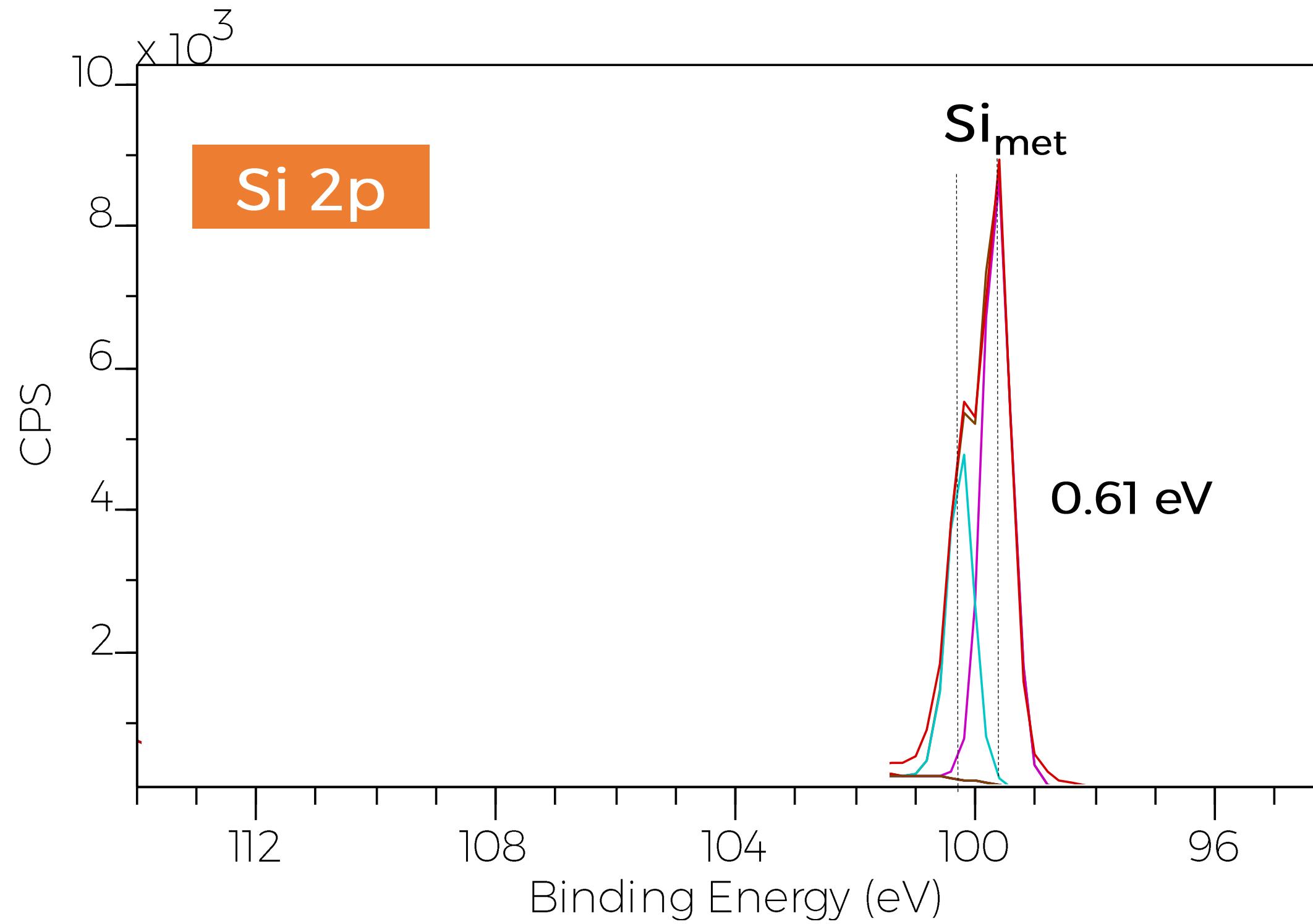
02 COMPOSICIÓN QUÍMICA

Identificación y cuantificación de estados químicos.

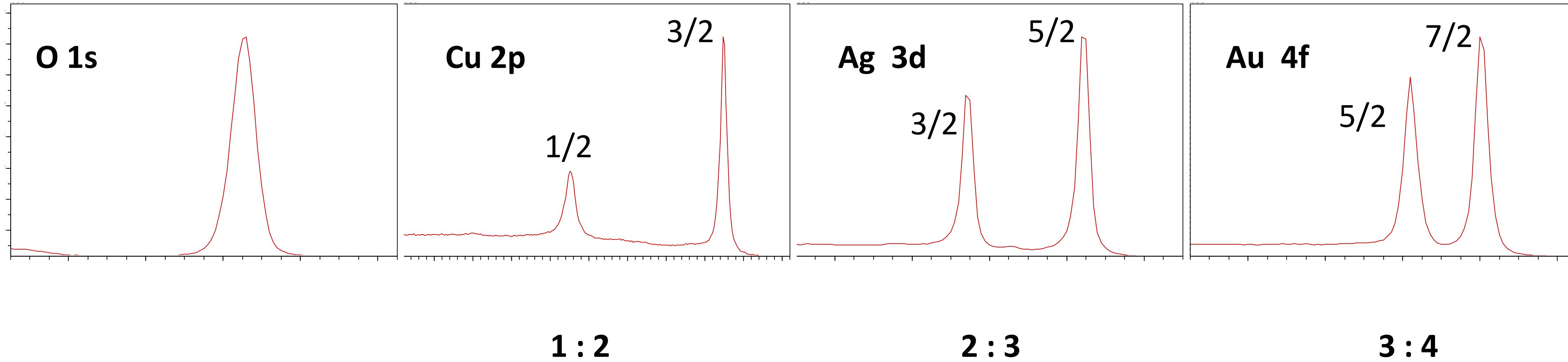
ESPECTROS Y SOFTWARE



SPIN-ORBIT SPLITTING



El **desdoblamiento** (splitting) ocurre debido a la **combinación** de los momentos orbital **angular** (l) y **magnético** del (s) y tiene dependencia en el número atómico z así como en el tipo de nivel profundo (p, d, f)



Nomenclature: nI_j

$$j = l \pm s$$

n principal quantum number

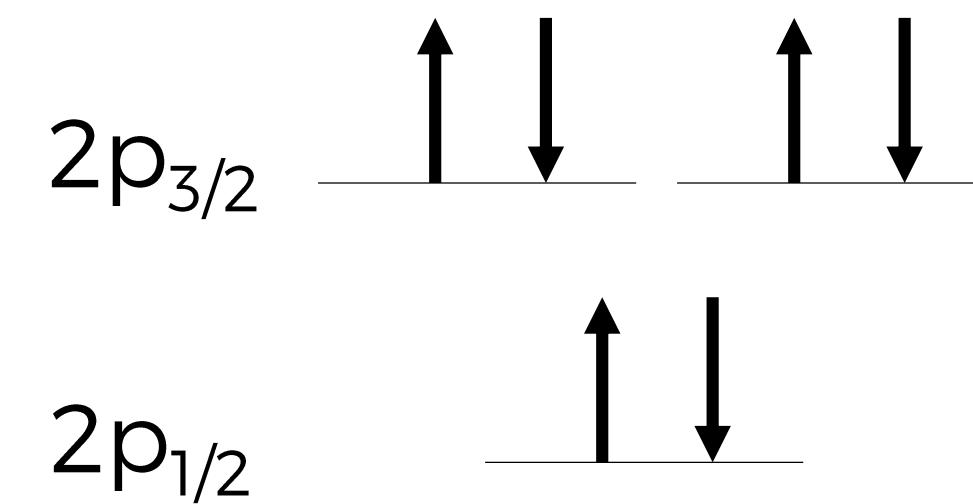
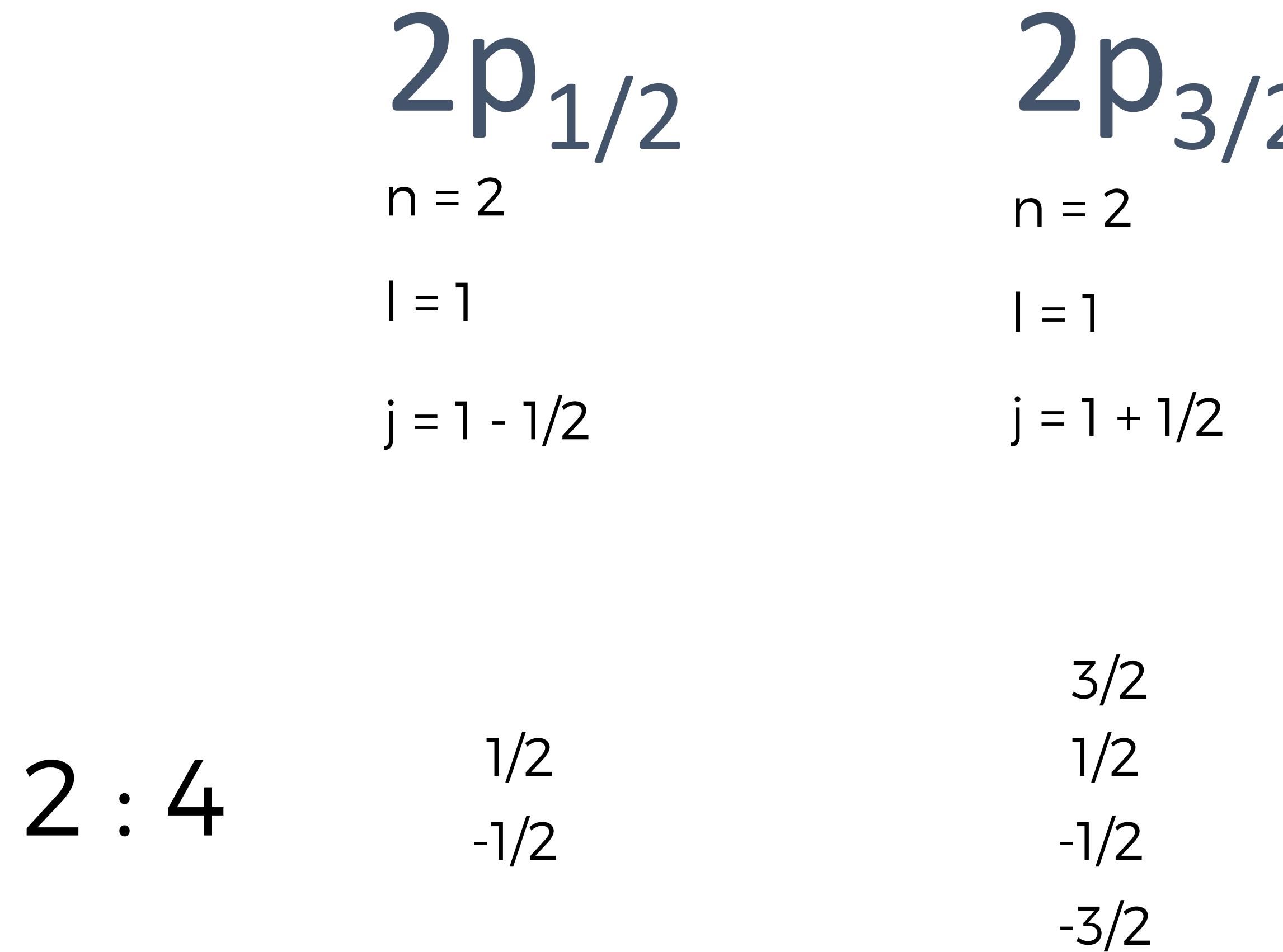
| angular momentum quantum number

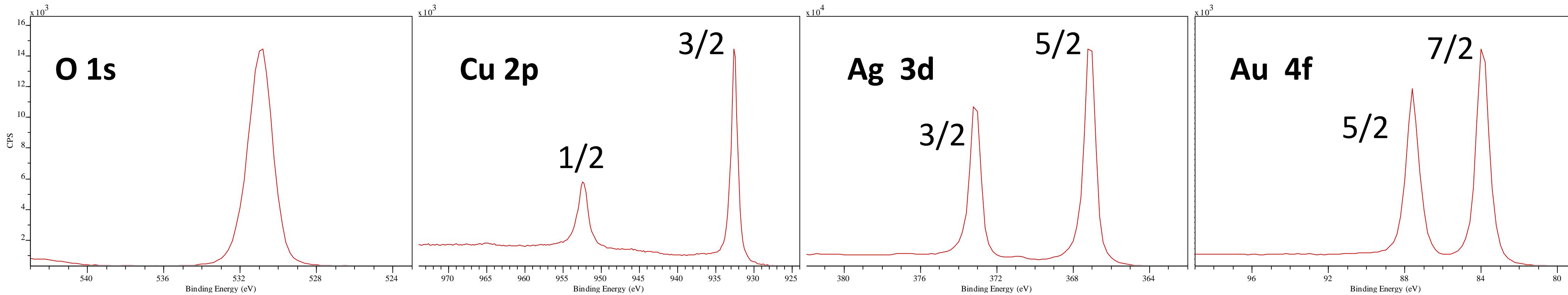
s spin angular momentum



$$j = l \pm s$$

RUSELL – SAUNDERS COUPLING APPROXIMATION





Singlet ($l = 0$)
 $j = \pm 1/2$

Doublet ($l = 1$)
 $j = 1\pm 1/2$

Doublet ($l = 2$)
 $j = 2\pm 1/2$

Doublet ($l = 3$)
 $j = 3\pm 1/2$

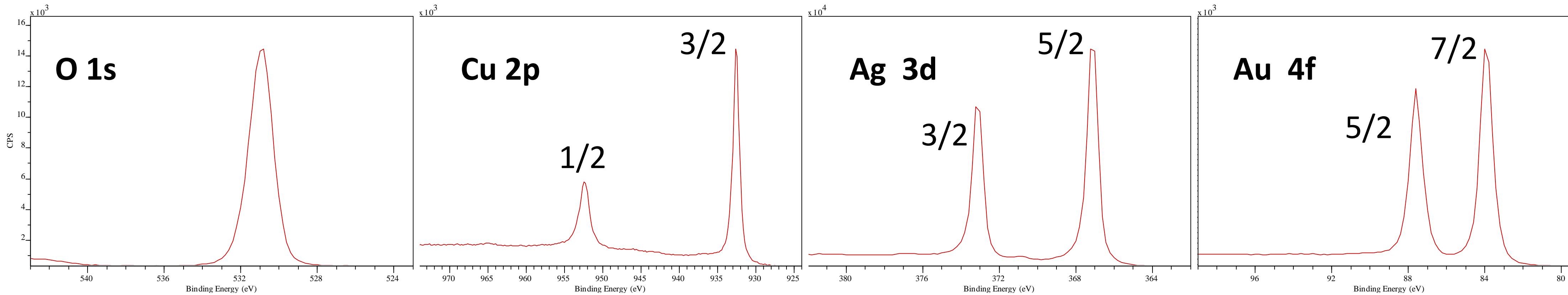
$1/2$
 $-1/2$

2:4
 $3/2$
 $1/2$
 $-1/2$
 $-1/2$
 $-3/2$

4:6
 $5/2$
 $3/2$
 $1/2$
 $-1/2$
 $-3/2$
 $-5/2$

$7/2$
 $5/2$
 $5/2$
 $3/2$
 $3/2$
 $1/2$
 $-1/2$
 $-3/2$
 $-5/2$
 $-7/2$





Singlet ($l = 0$)
 $j = \pm 1/2$

Doublet ($l = 1$)
 $j = 1\pm 1/2$

Doublet ($l = 2$)
 $j = 2\pm 1/2$

Doublet ($l = 3$)
 $j = 3\pm 1/2$

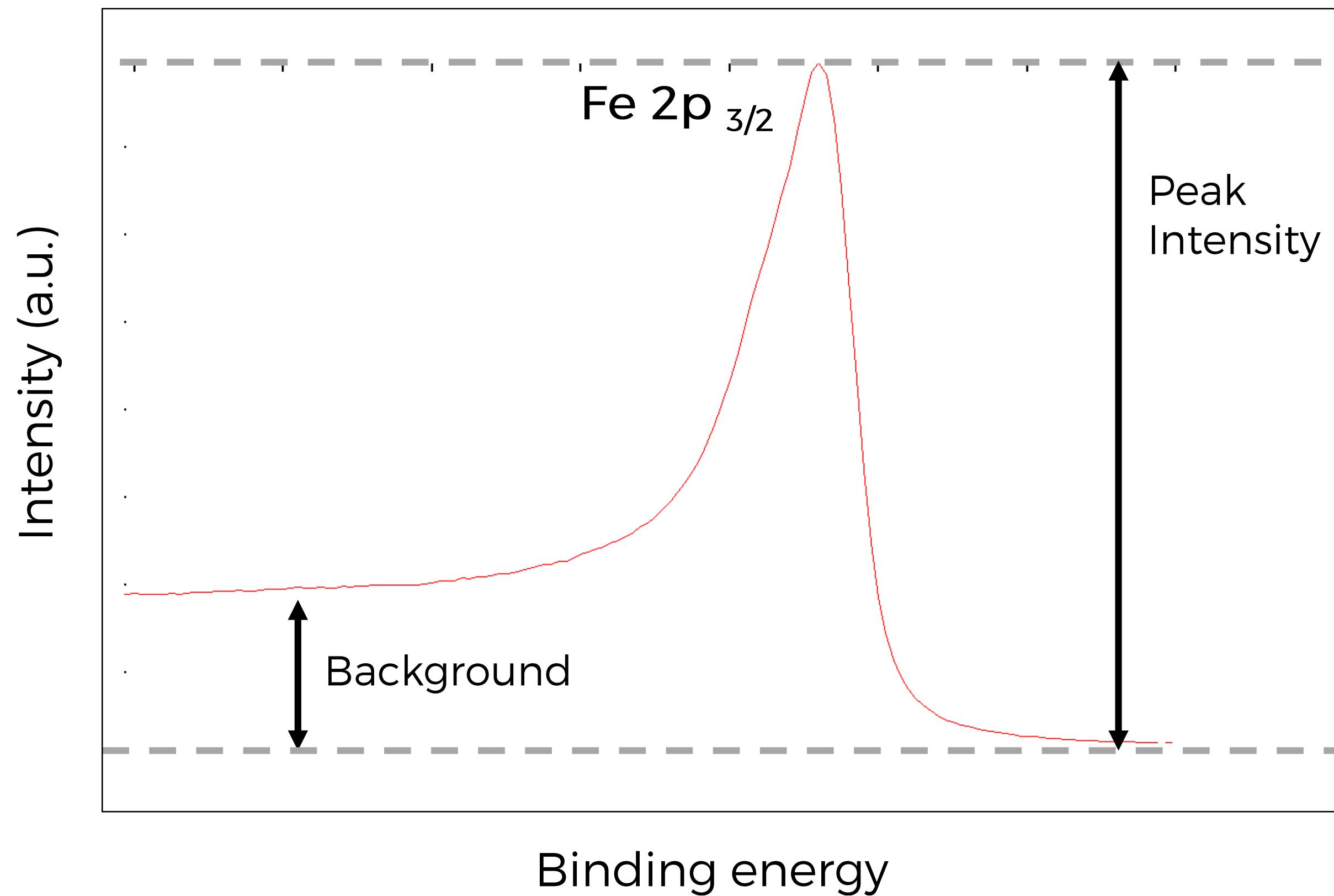
1/2
-1/2

0.5
1/2 1/2
-1/2 -1/2
 -3/2

3/2	3/2	5/2
1/2	1/2	5/2
-1/2	-1/2	3/2
-3/2	-3/2	3/2
-5/2		1/2

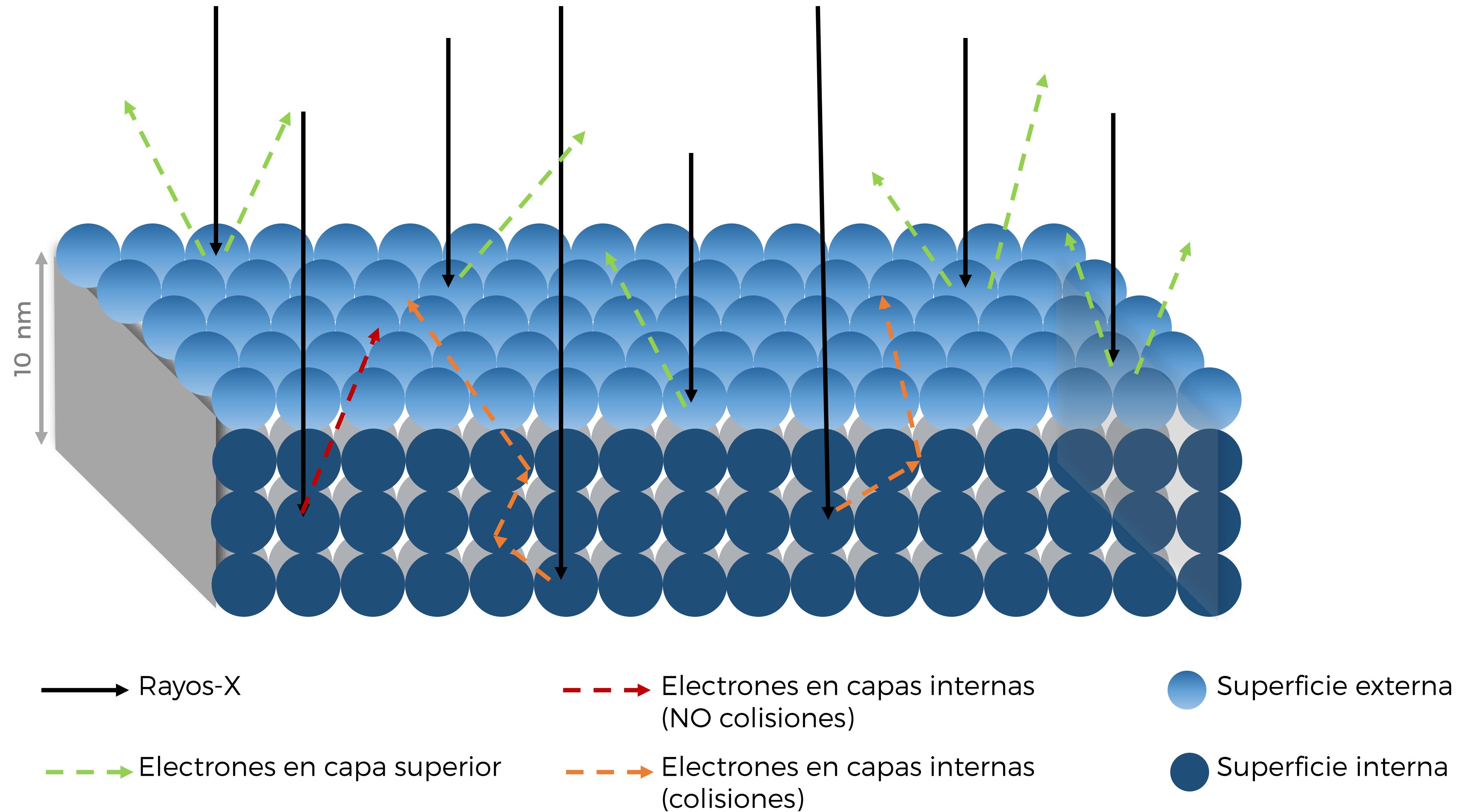
7/2	5/2	5/2
3/2	3/2	3/2
1/2	1/2	1/2
-1/2	-1/2	-1/2
-3/2	-3/2	-3/2
-5/2	-5/2	-5/2
-7/2		-7/2

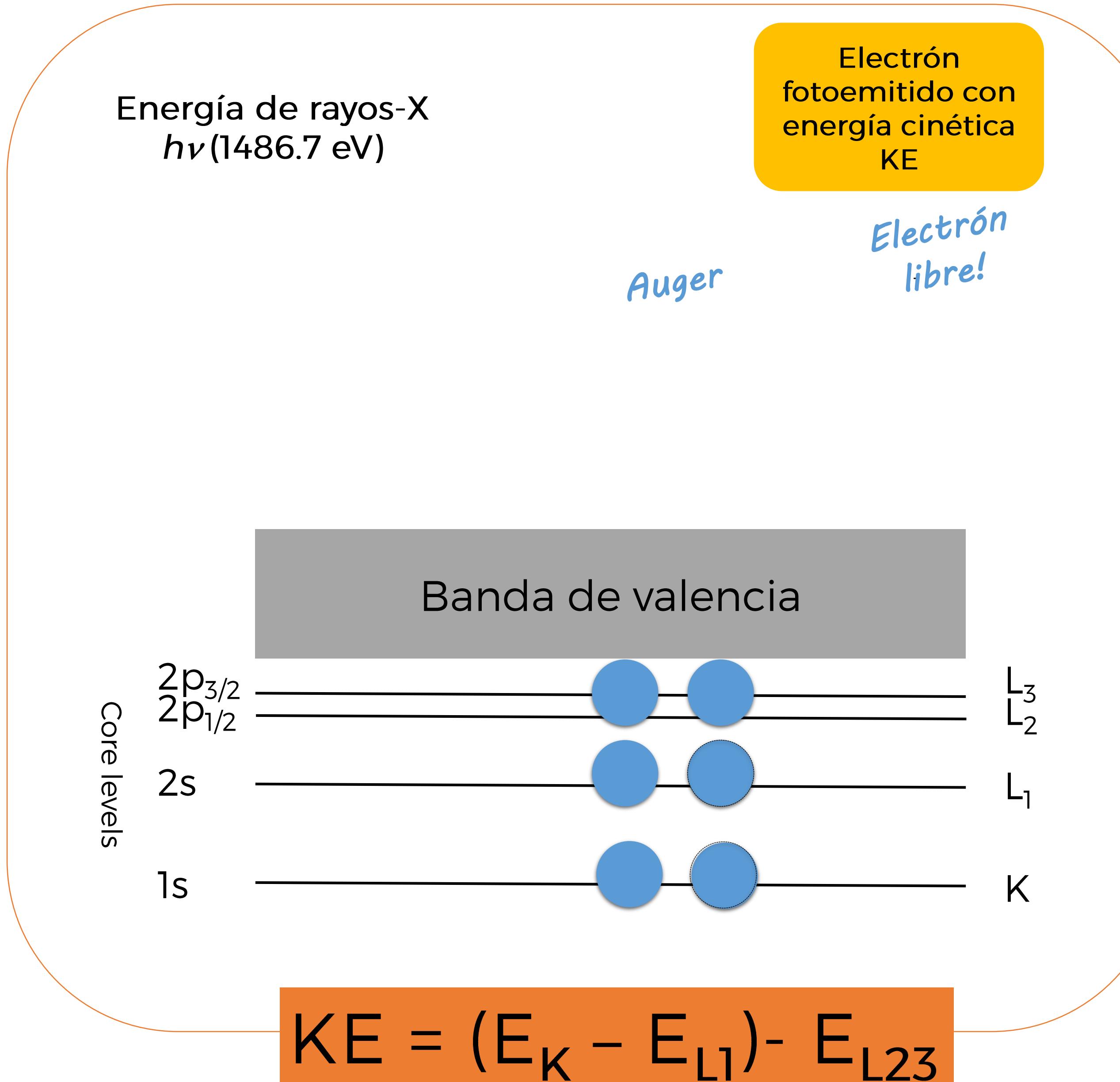




El *background* está formado por fotoelectrones que perdieron energía por dispersión inelástica durante un proceso de tres pasos: 1) la excitación del fotoelectrón; 2) El transporte del fotoelectrón desde el sólido a la superficie; y 3) la emisión del fotoelectrón en el vacío.

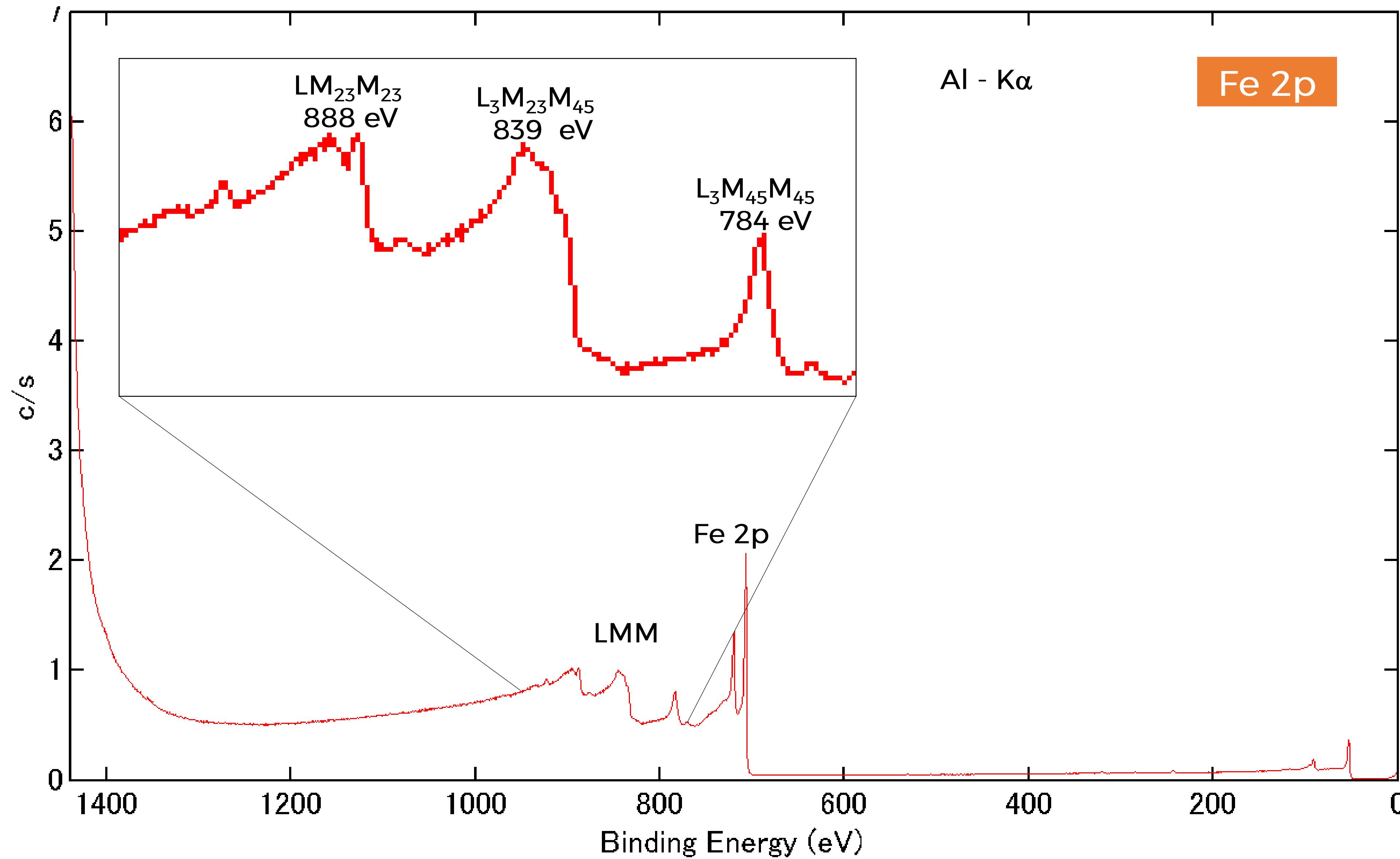
Entonces, el *background* es la *representación* de los fotoelectrones que *pierden* energía durante este proceso de tres pasos. Las pérdidas de energía pueden clasificarse en pérdidas *intrínsecas* (eventos dentro del átomo) y pérdidas *extrínsecas* (eventos en la estructura cristalina)

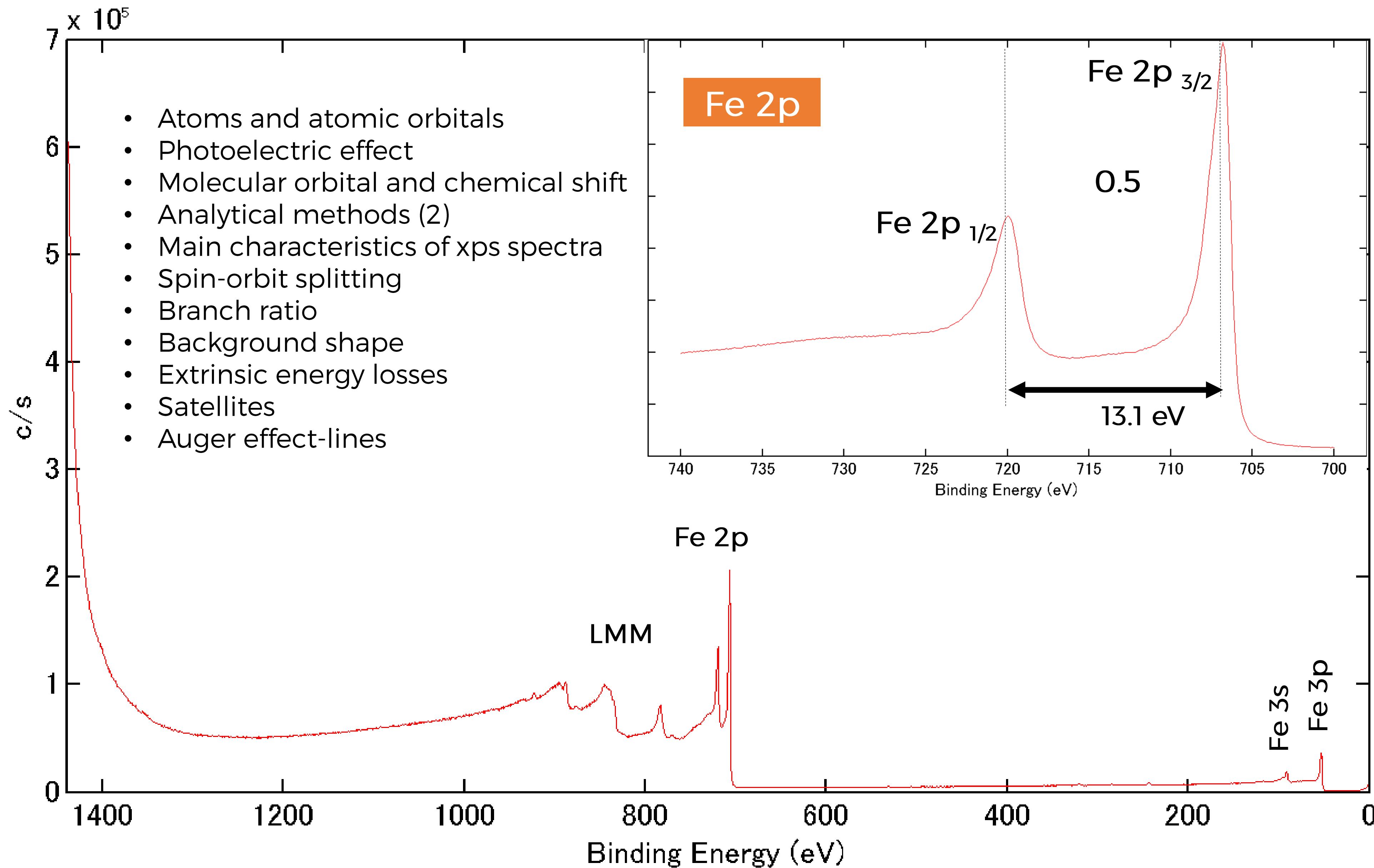


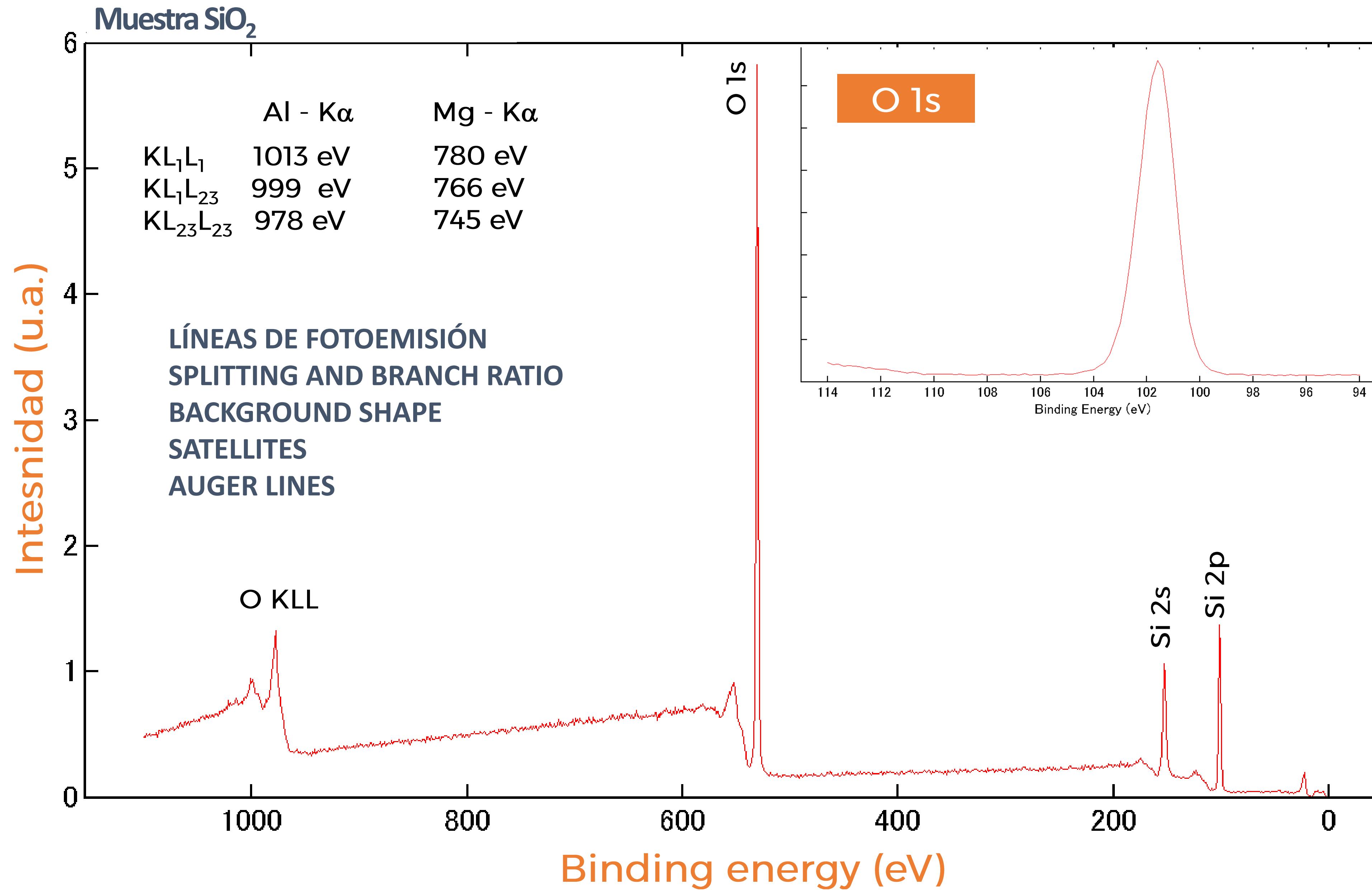


$E_K - E_{L1}$ energía ganada por la aniquilación core-hole.

E_{L23} energía necesaria para romper con la energía de enlace de un electrón Auger.

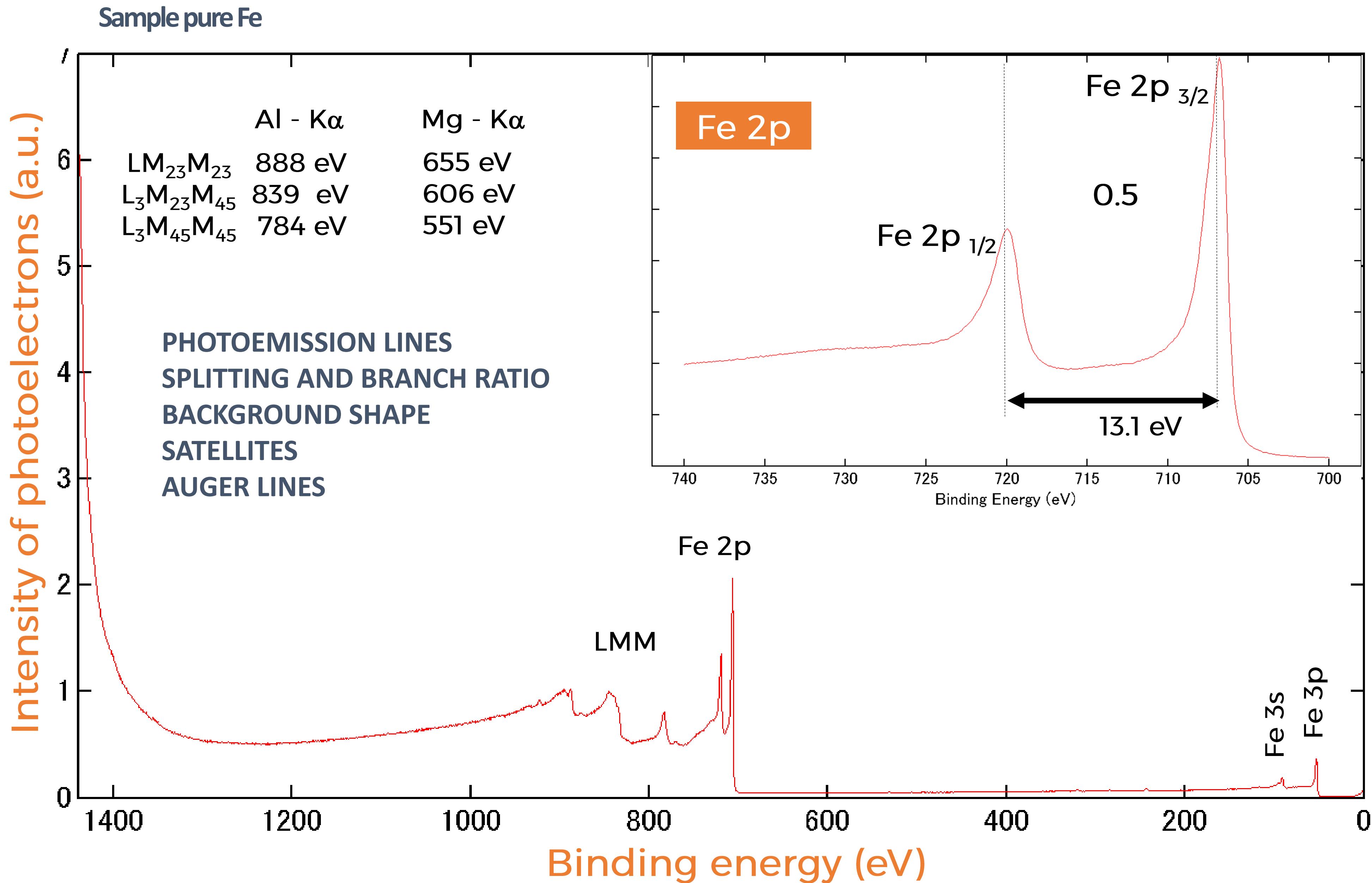


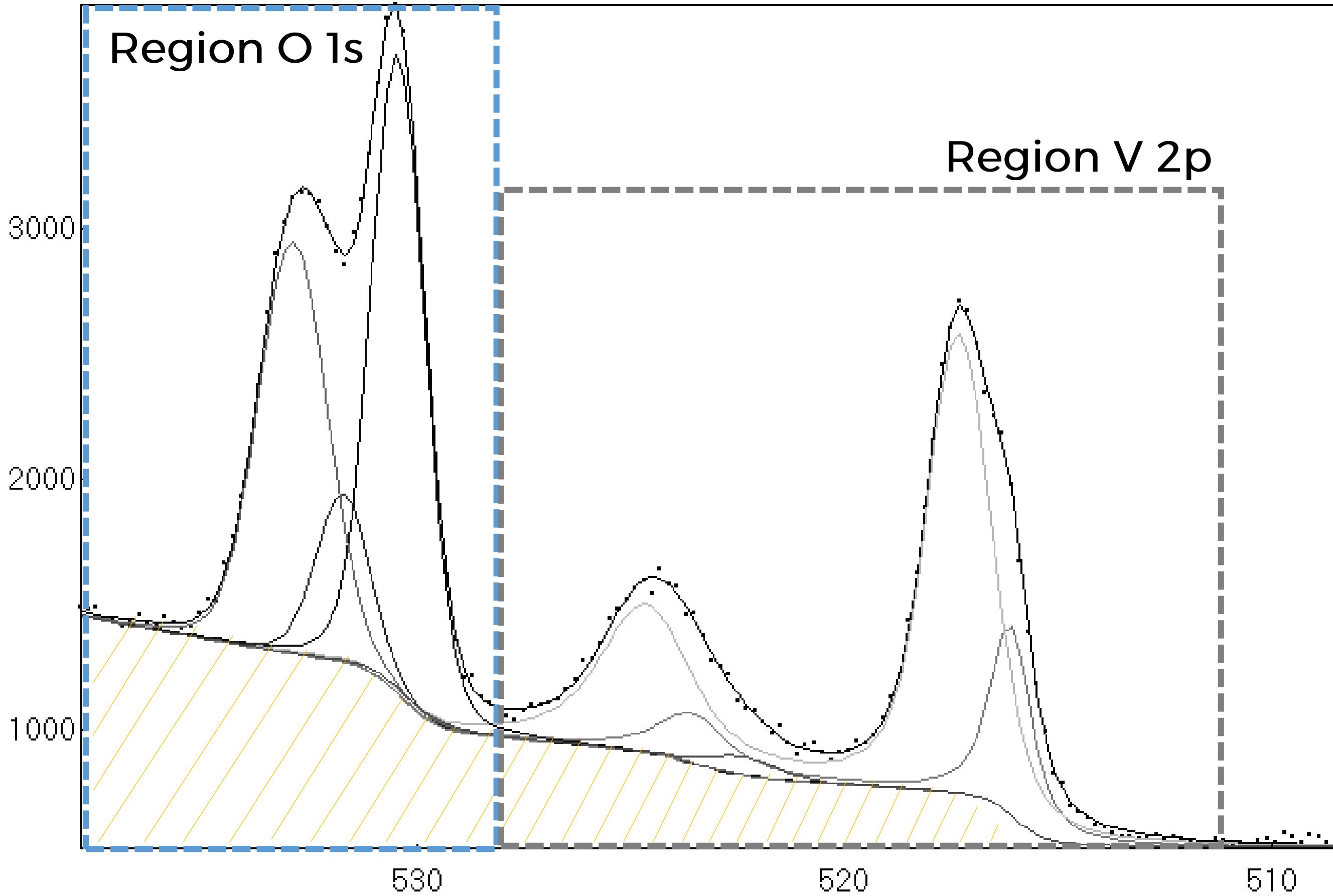




FUNDAMENTS

PRINCIPALES CARACTERÍSTICAS DEL ESPECTRO DE XPS

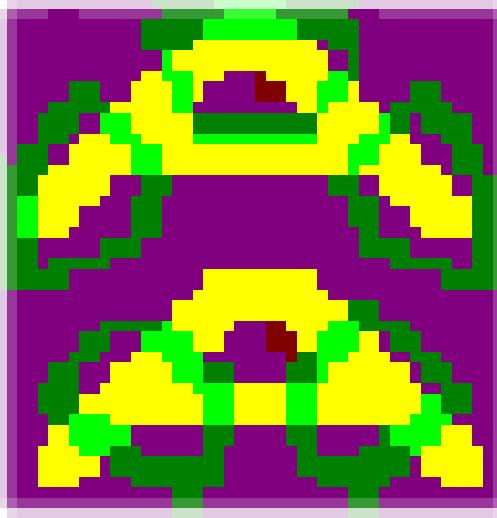




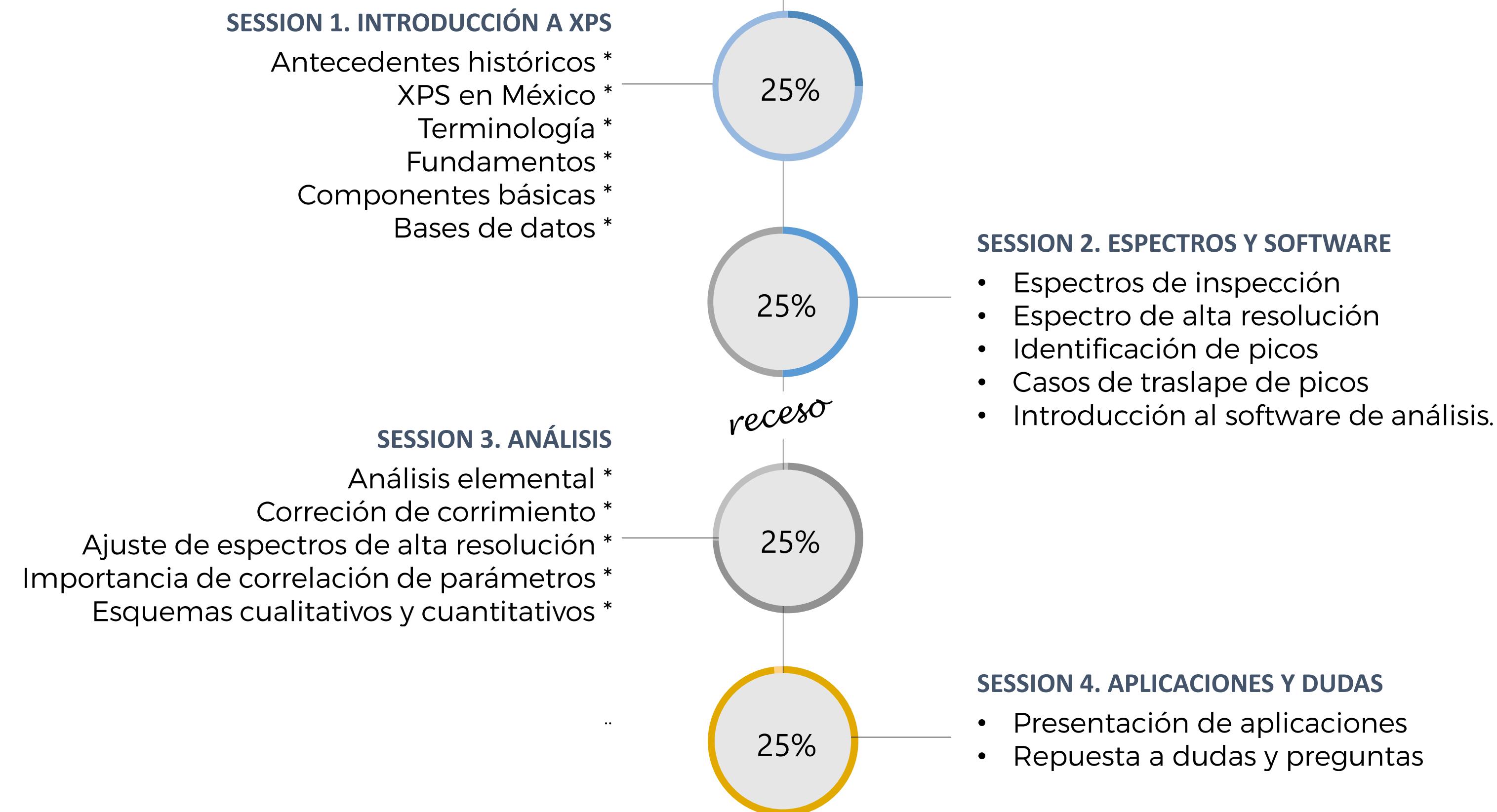
As the background comes from different core levels in the spectra with overlapped peaks, then different values of background must be assigned. This is possible using the background Shirley-Vegh-Salvi-Castle.

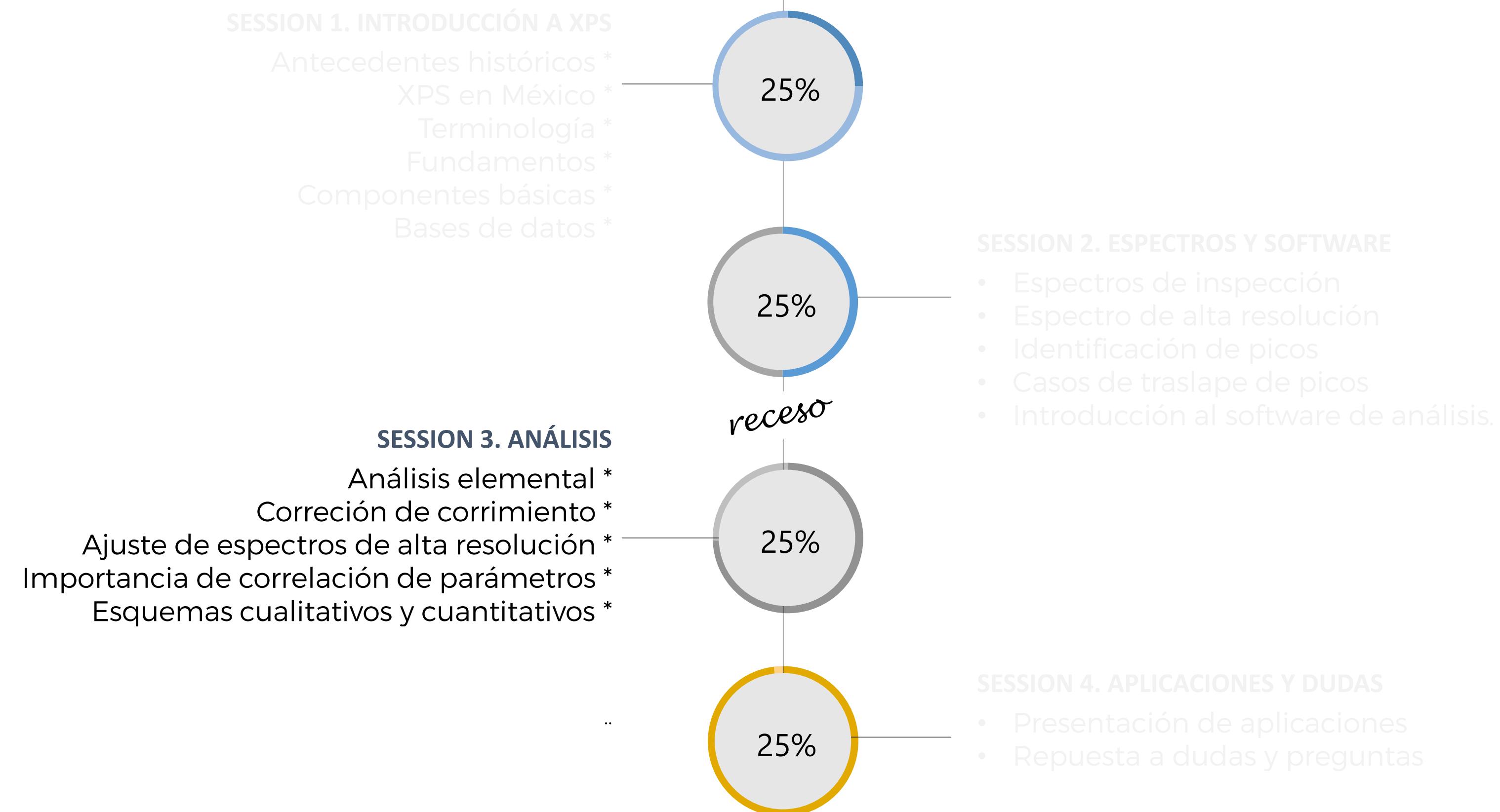


www.casaxps.com



www.rdataa.com/aanalyzer/aanaHome.htm





CasaXPS

FITTING METHODS

BACKGROUND MODELING

Is used to remove the inelastically scattered electrons form the XPS spectrum. The models includes: Shirley-Vegh-Salvi-Castle, Shirley - Sherwood, slope, Shirley, Tougaard and Linear background.

$$B_n(E) = k_n \int_E^{E_\infty} dE' [I(E') - B_{n-1}(E')] \quad \text{Shirley-Sherwood}$$

$$\frac{dB_S(E)}{dE} = -k_S \int_{E+\Delta}^{E_{\text{right}}} dE' [I(E') - I_{\text{right}}] \quad \text{Slope}$$

$$B_2(E) = k_2 \int_E^{E_{\text{right}}} dE' [I(E') - I_{\text{right}} - B_1(E')] \quad \text{Shirley}$$

$$B_{2P-T}(E) = \int_E^{E_{\text{right}}} dE' \frac{B(E'-E)}{\left[(E'-E)^2 + C\right]^2} [I(E') - I_{\text{right}}] \quad \text{Tougaard}$$

Linear

01

02

CURVE FITTING

Describes the form of the spectra line-shape and can be modeled using: Lorentzian, Gaussian, Voight, Doniach-Sunjic and Double Lorentzian.

Lorentzian

$$L(x; F, E, h) = \left[\frac{h}{1+4 \frac{(x-E)^2}{F^2}} \right]$$

Gaussian

$$G(x; F, E, h) = h * \exp \left[-4 \ln 2 \frac{(x-E)^2}{F^2} \right]$$

Voigt

$$h(x) = f(x) * g(x) = \int_{-\infty}^{\infty} f(u) g(x-u) du$$

Doniach-Sunjic

$$I(E) \sim \frac{\cos \left[\frac{\pi \alpha}{2} + (1-\alpha) \arctan \frac{E-E_0}{\gamma} \right]}{\left[(E-E_0)^2 + \gamma^2 \right]^{\frac{1-\alpha}{2}}}$$

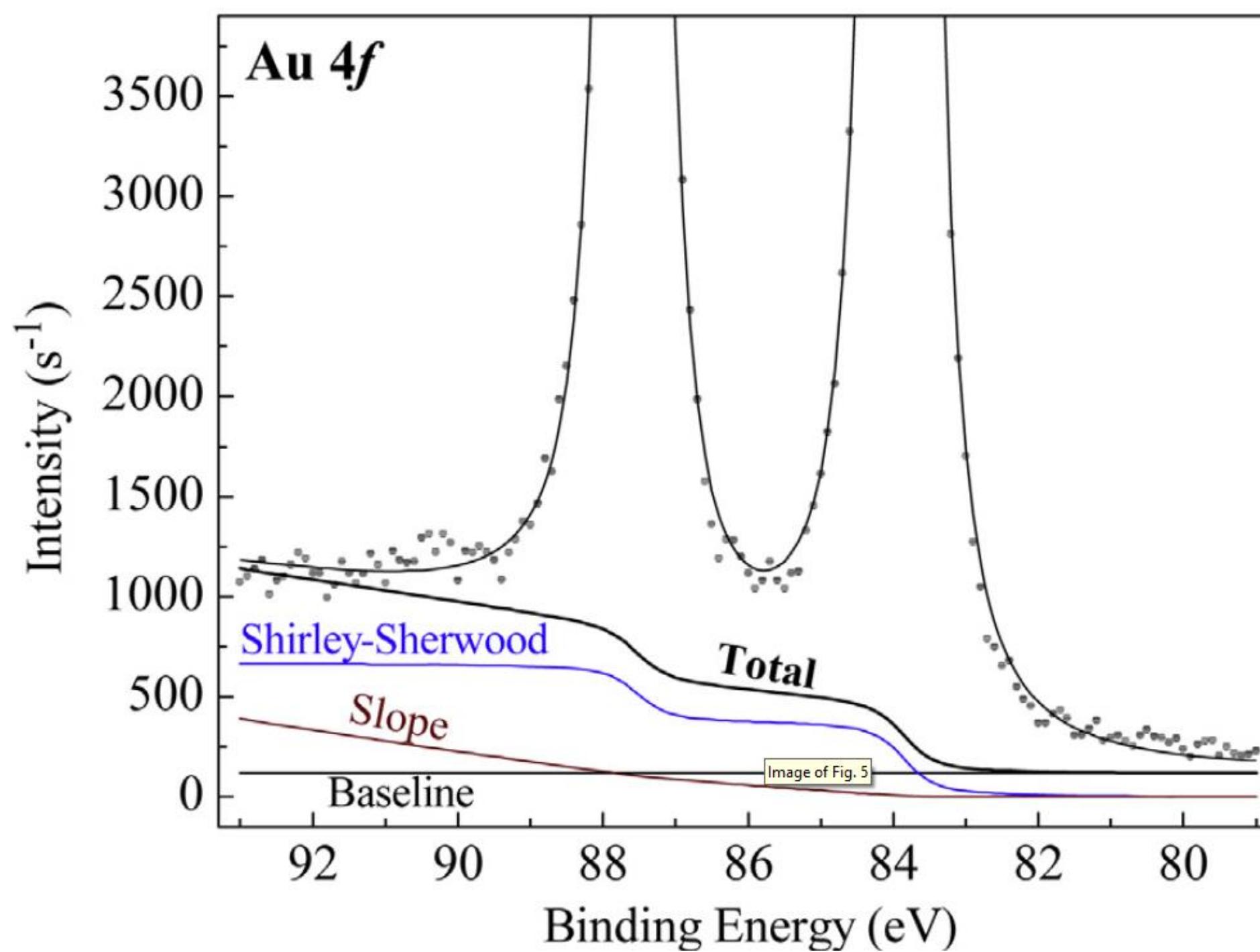
Double Lorentzian

FITTING METHODS

XPS DECONCOLUTION PHASES

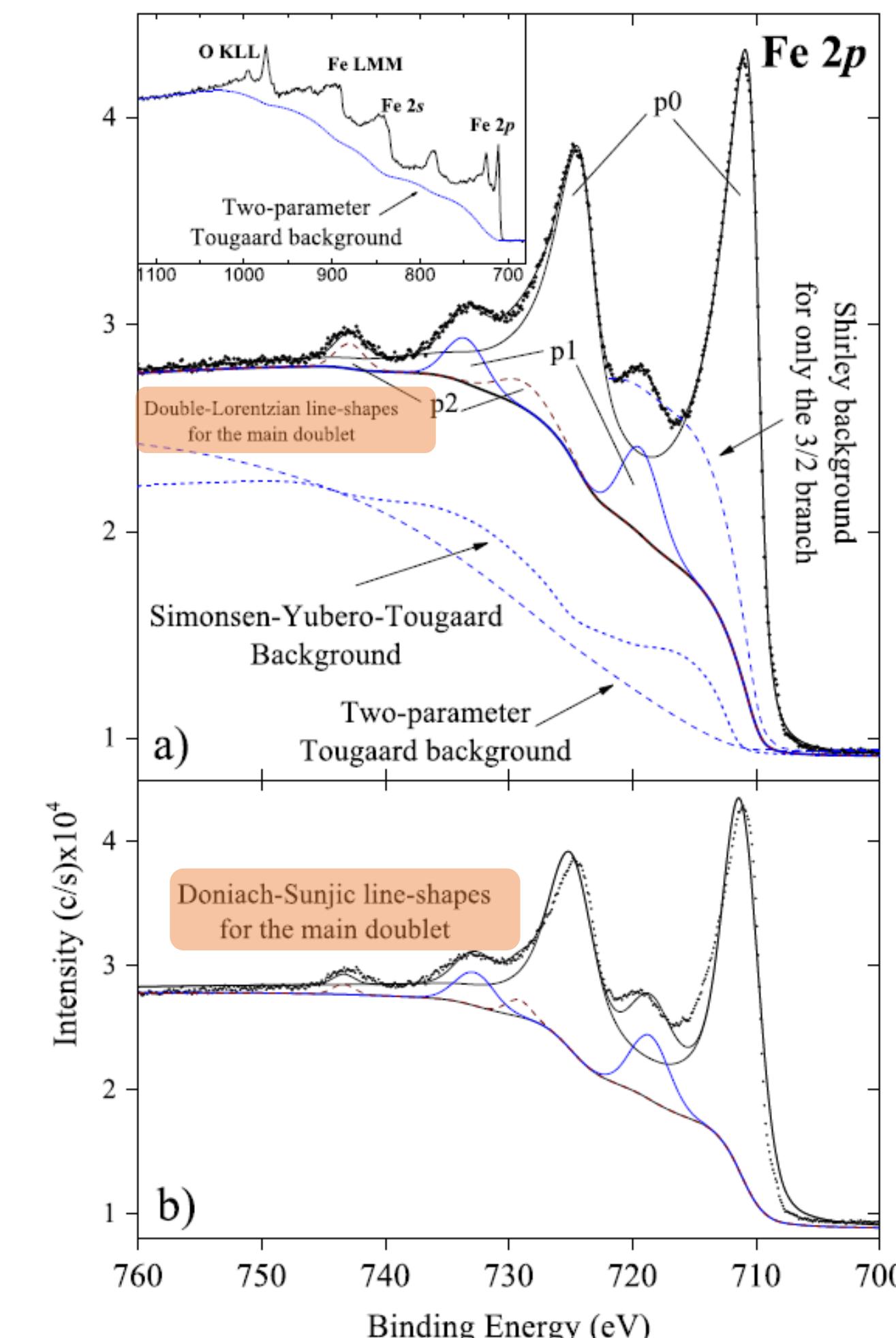
BACKGROUND MODELING 01

Is used to remove the inelastically scattered electrons form the XPS spectrum. The models includes: Shirley-Vegh-Salvi-Castle, Shirley - Sherwood, slope, Shirley, Tougaard and Linear background.



CURVE FITTING 02

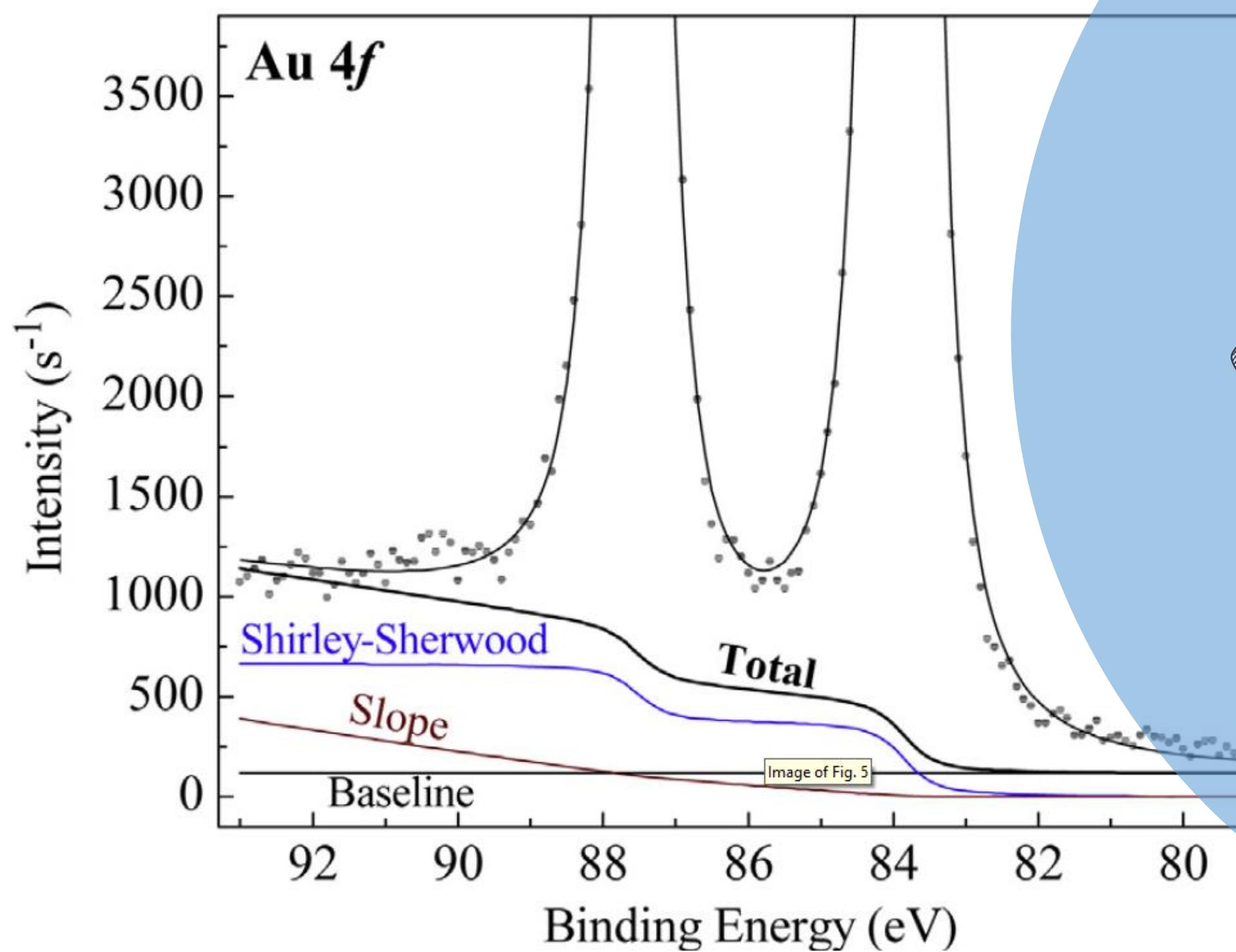
Describes the form of the spectra line-shape and can be modeled using: Lorentzian, Gaussian, Voight, Doniach-Sunjic and Double Lorentzian.



FITTING METHODS

BACKGROUND MODELING

Is used to remove the inelastically scattered electrons from the XPS spectrum. The models includes: Shirley-Vegh-Salvi-Castle, Shirley - Sherwood, slope, Shirley, Tougaard and Linear background.

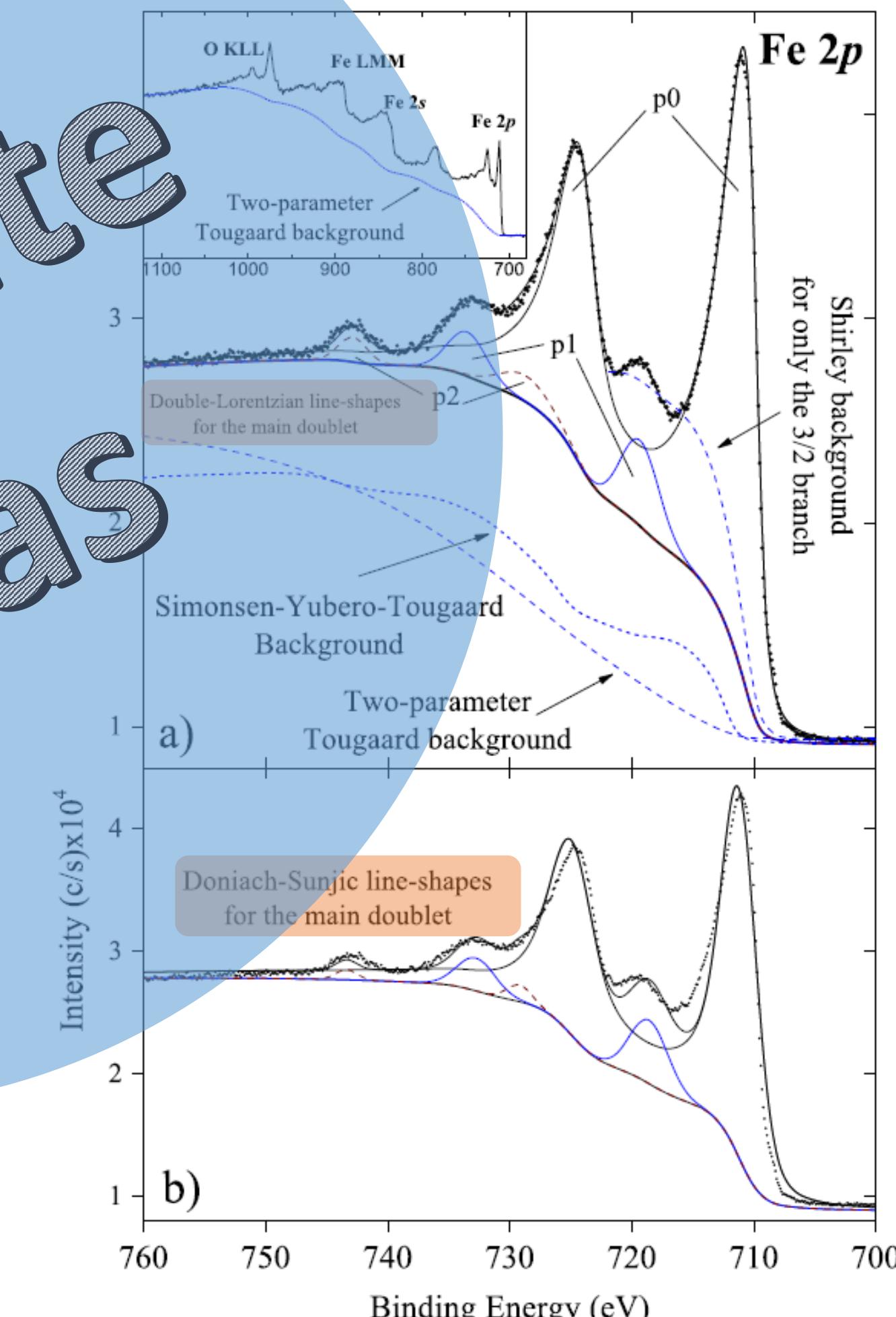


01

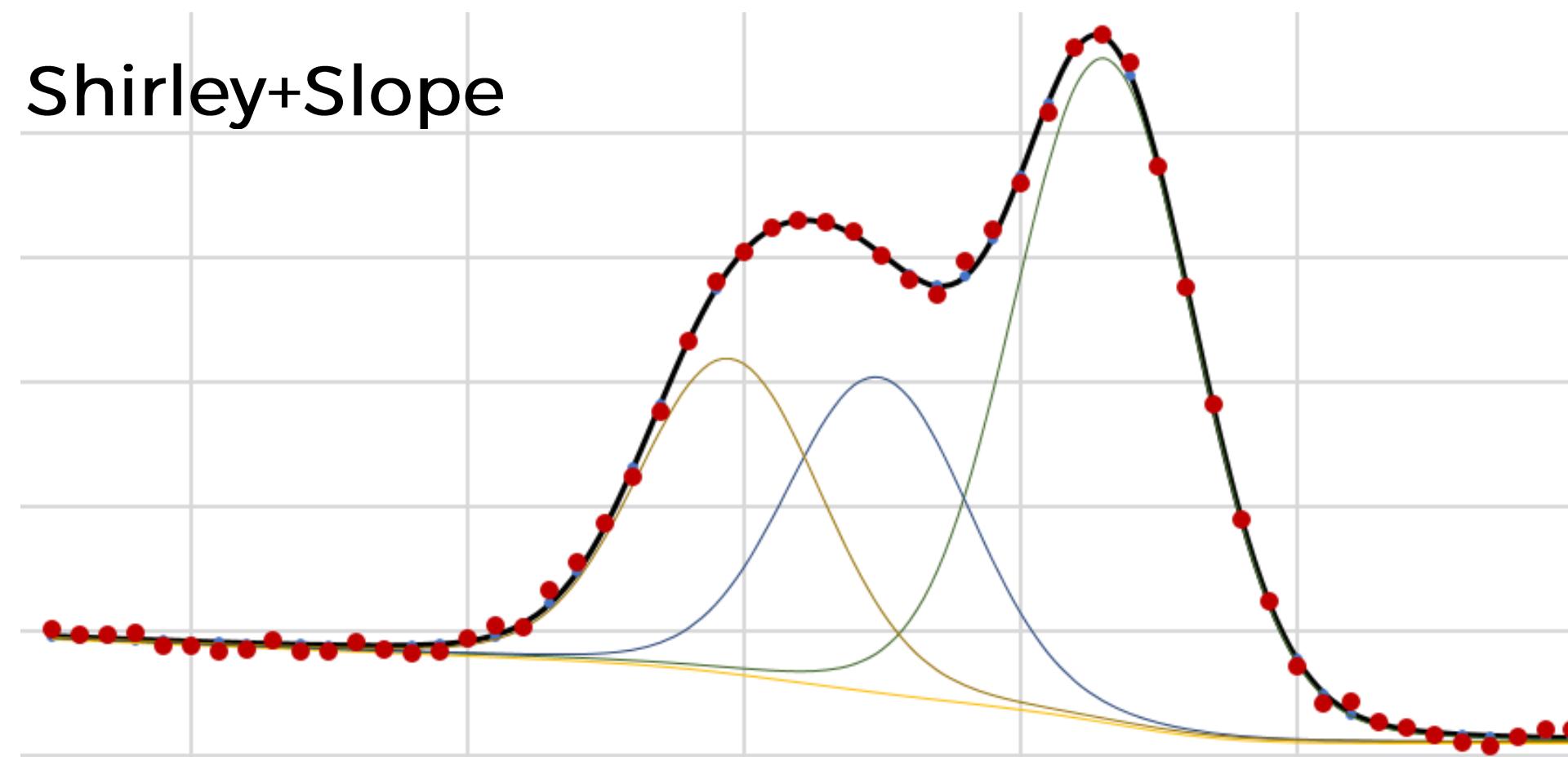
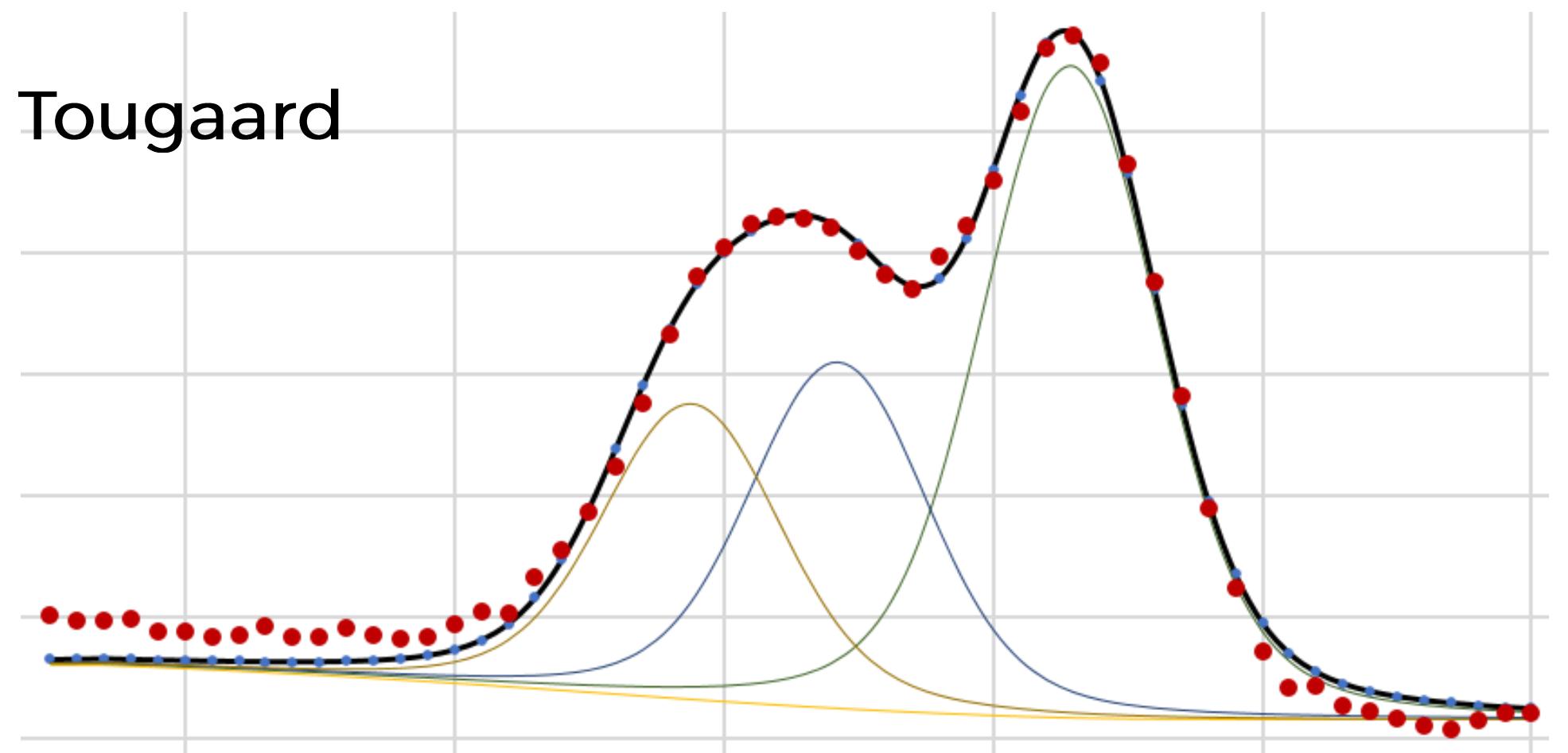
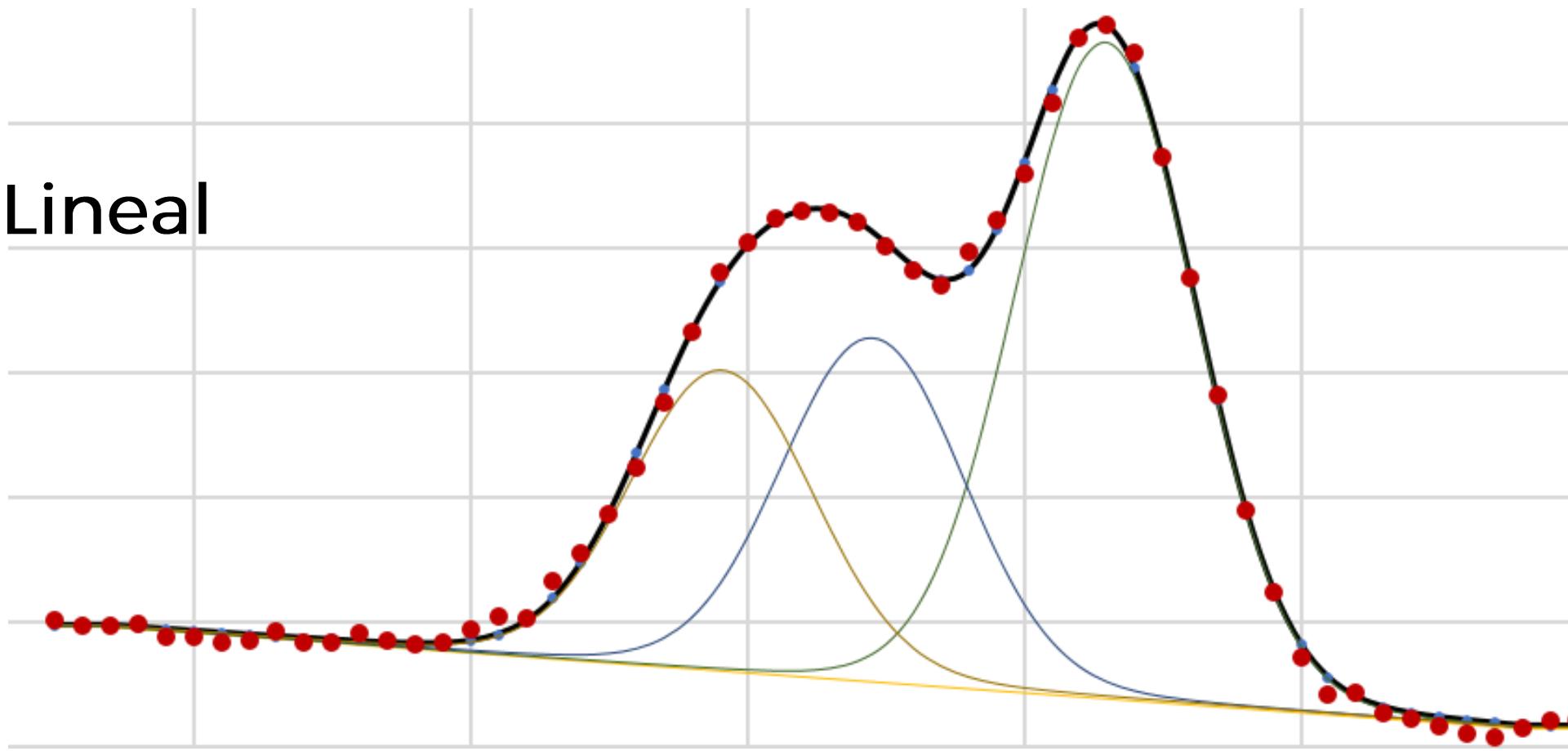
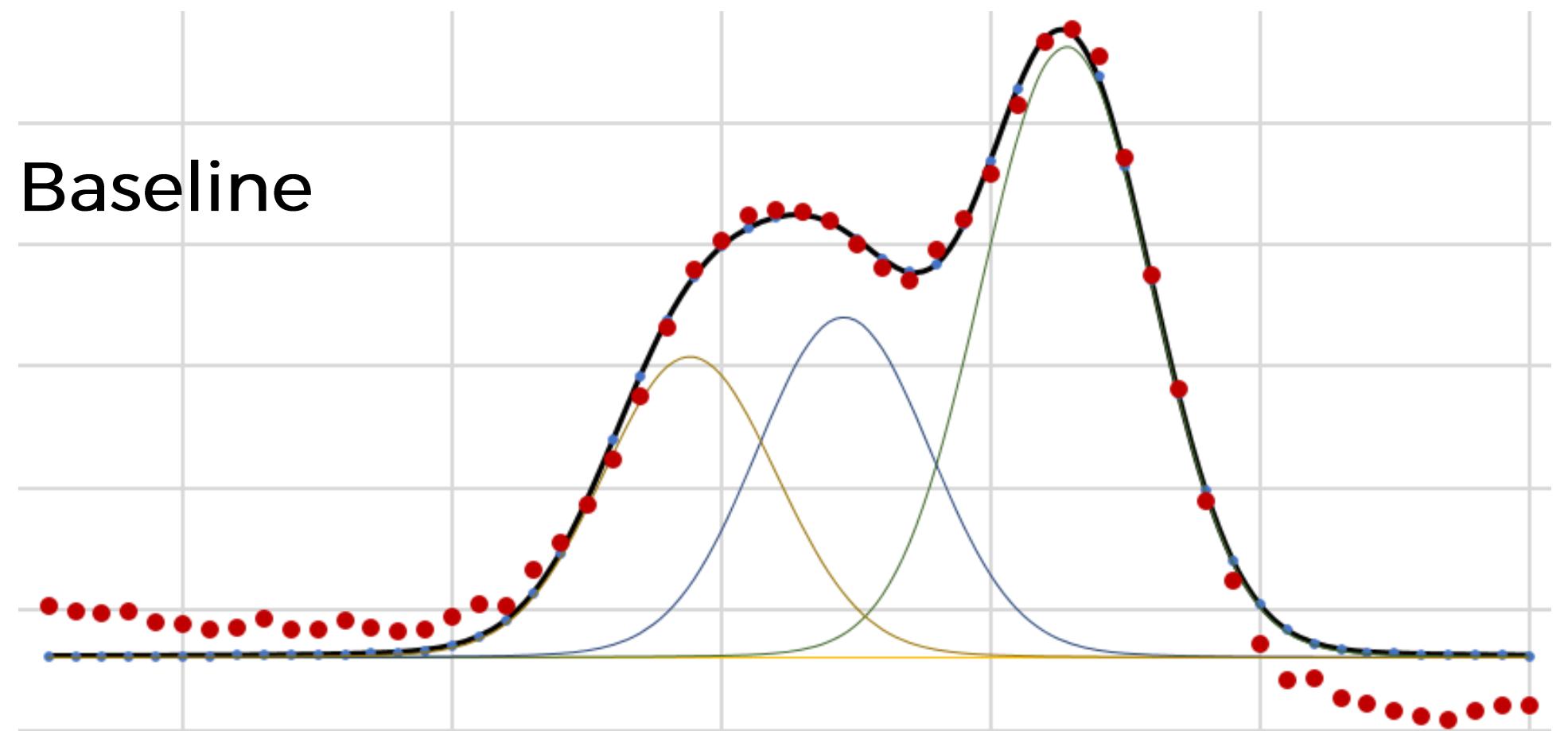
CURVE FITTING

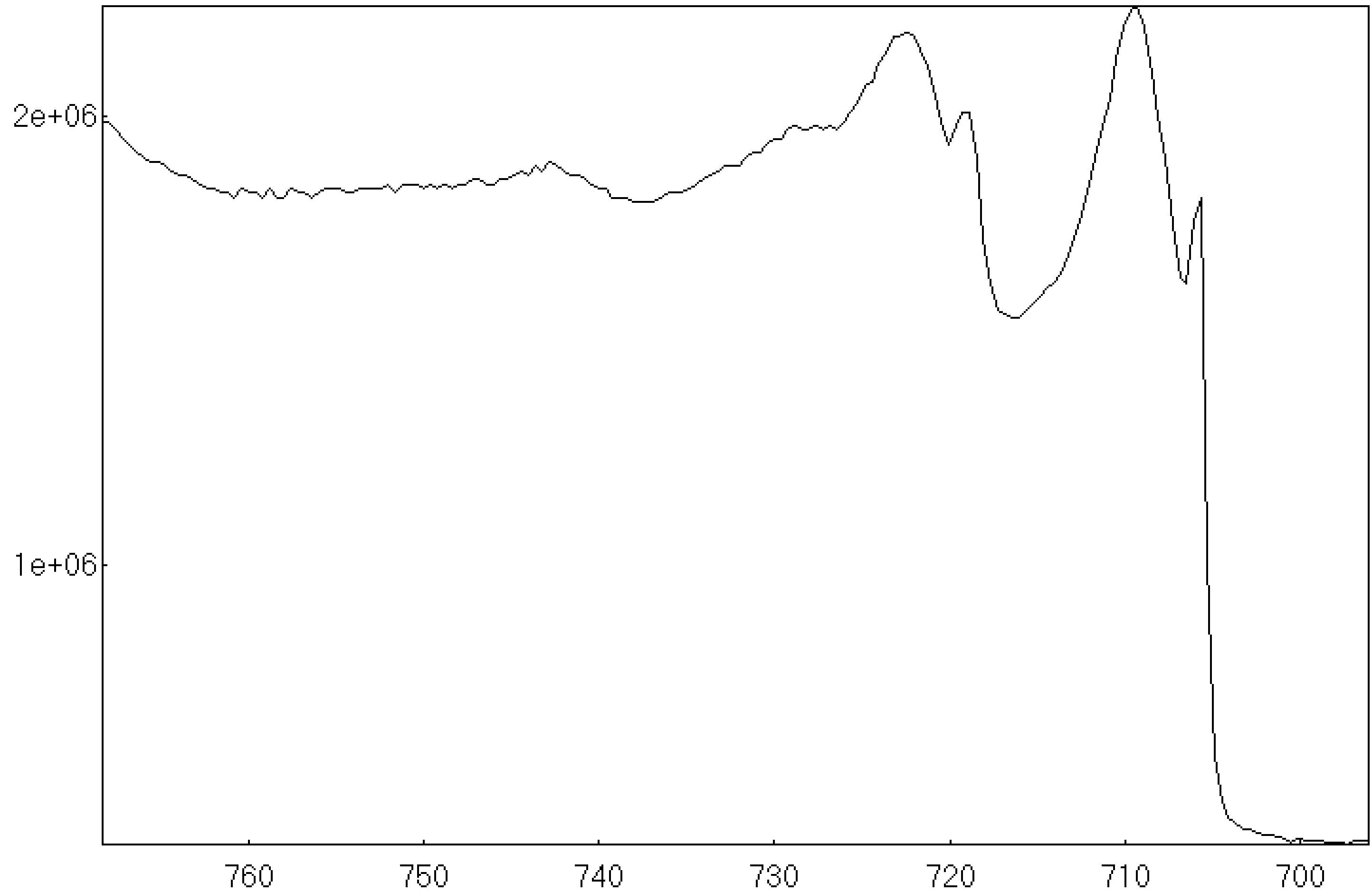
Describes the form of the spectra line-shape and can be modeled using: Lorentzian, Gaussian, Voight, Doniach-Sunjic and Double Lorentzian.

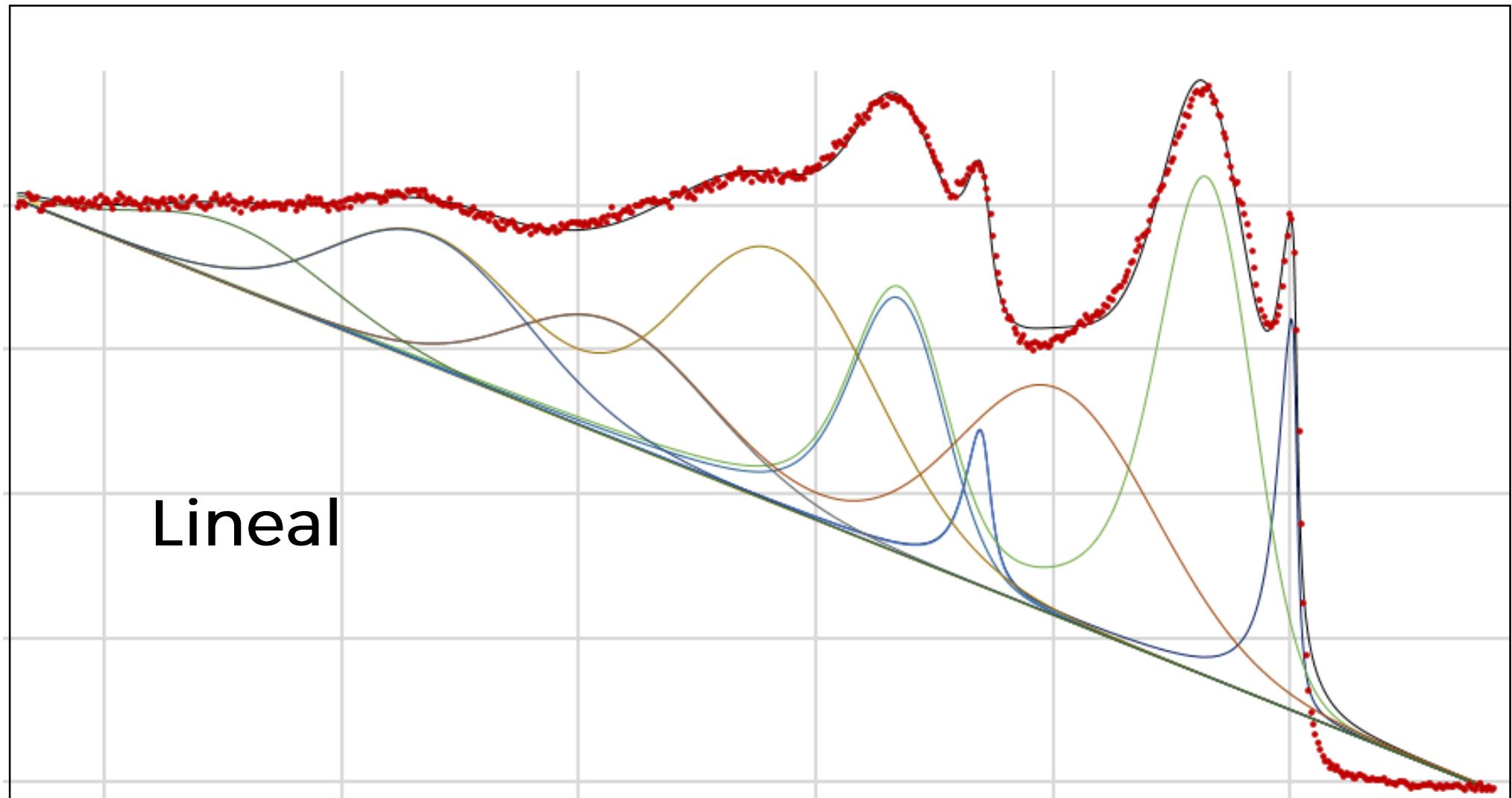
accurate areas



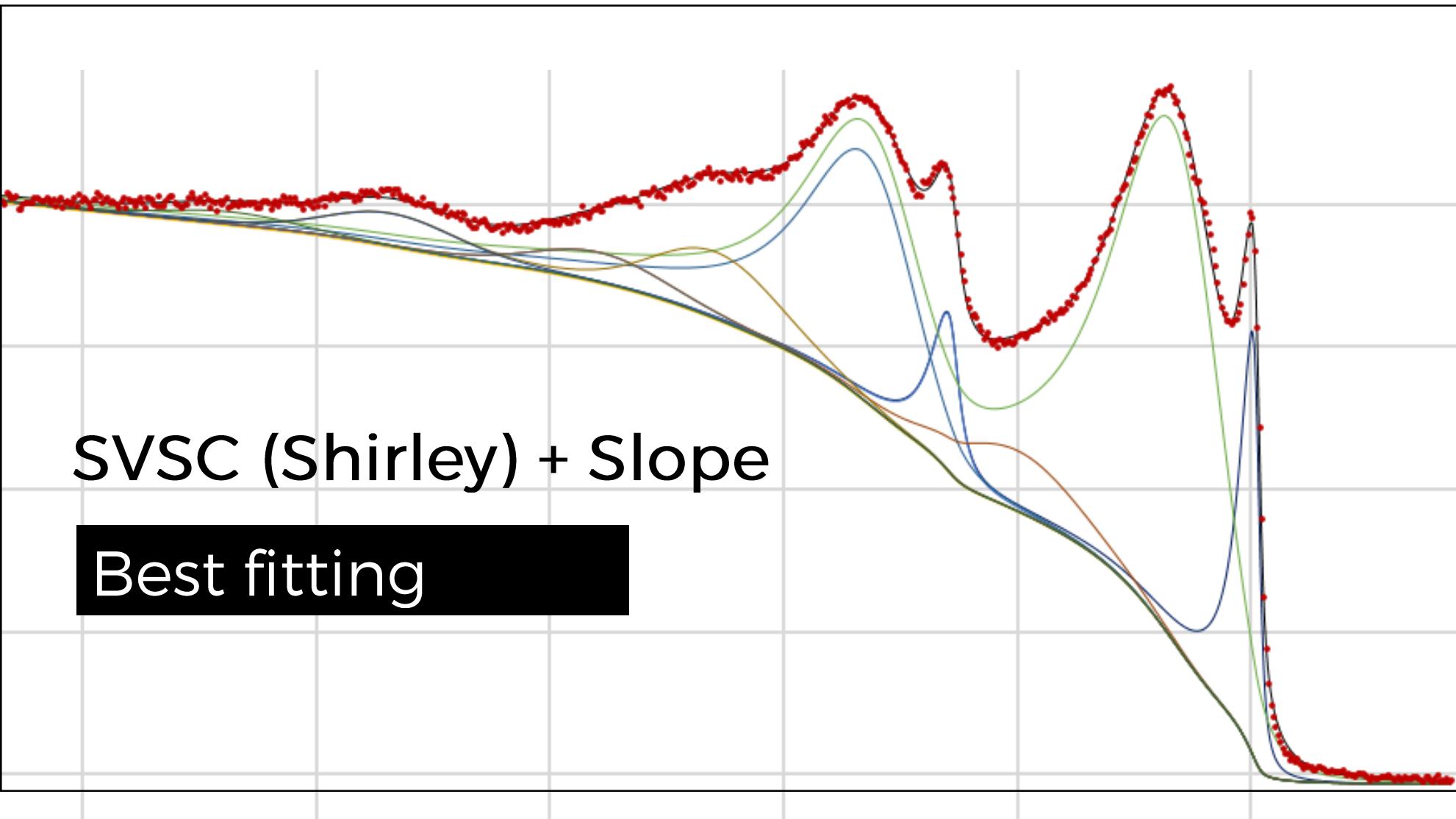
02





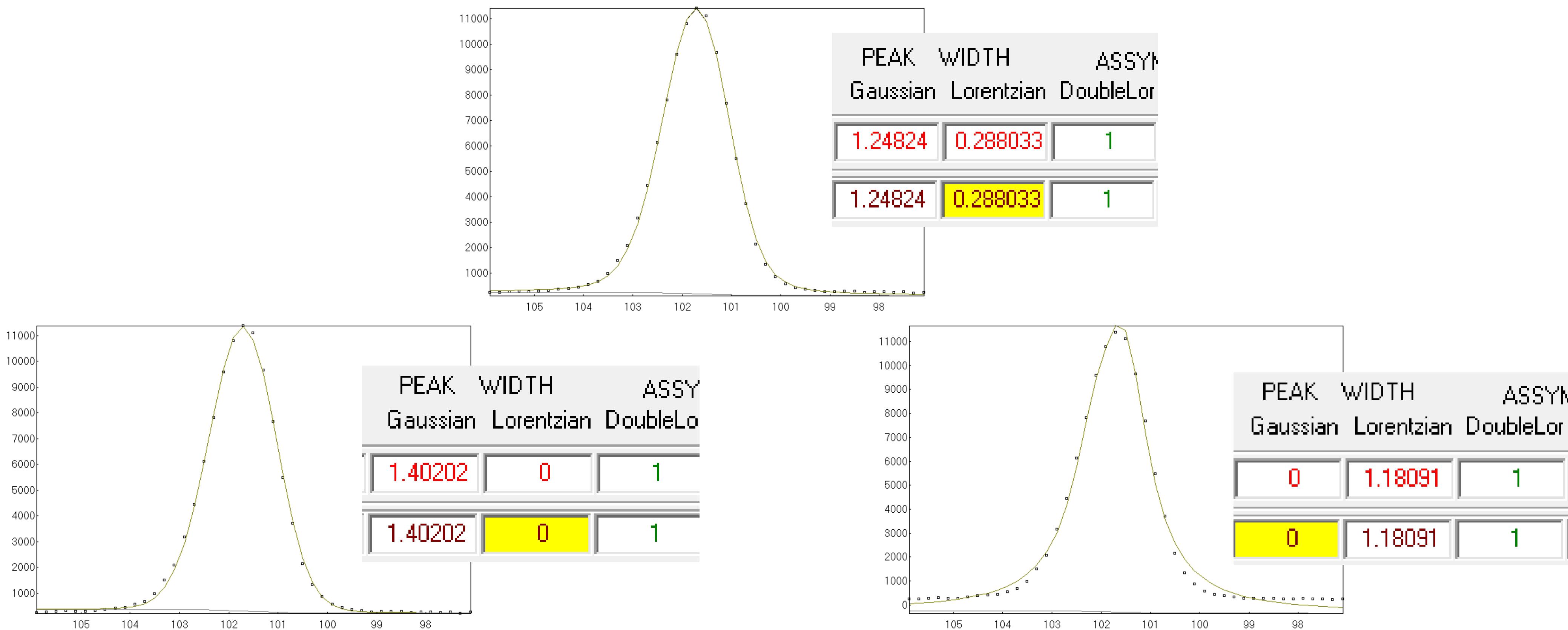


Lineal

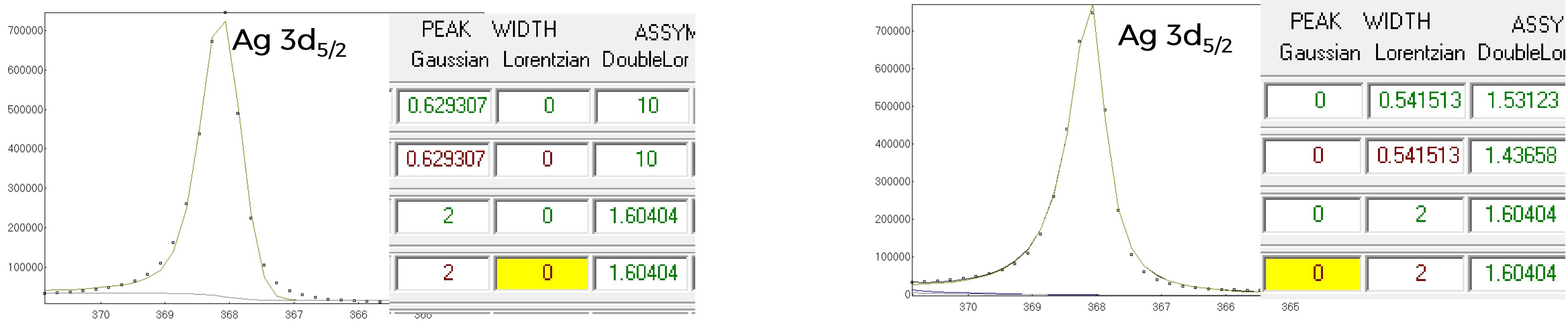
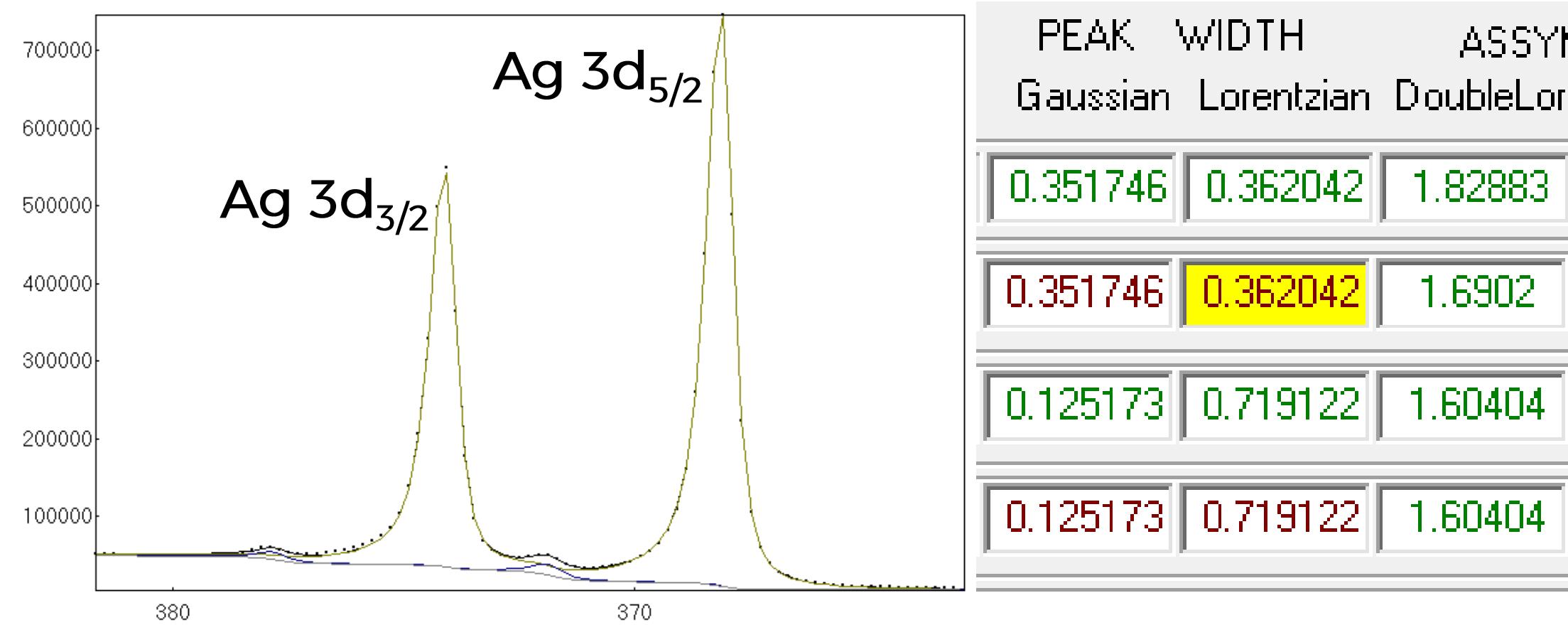


SVSC (Shirley) + Slope
Best fitting

The sum of backgrounds consider the contribution from intrinsic and extrinsic energy losses



A convolution of Gaussian and Lorentzian line-shapes is called Voigt. Both types of distributions are always present in different ratio in a photoemission event. Then, both must be considered if a symmetric line-shape is required.
 Symmetric peaks can be found in the polymer components of C1s, sp^3 bond in C1s and insulating oxides.

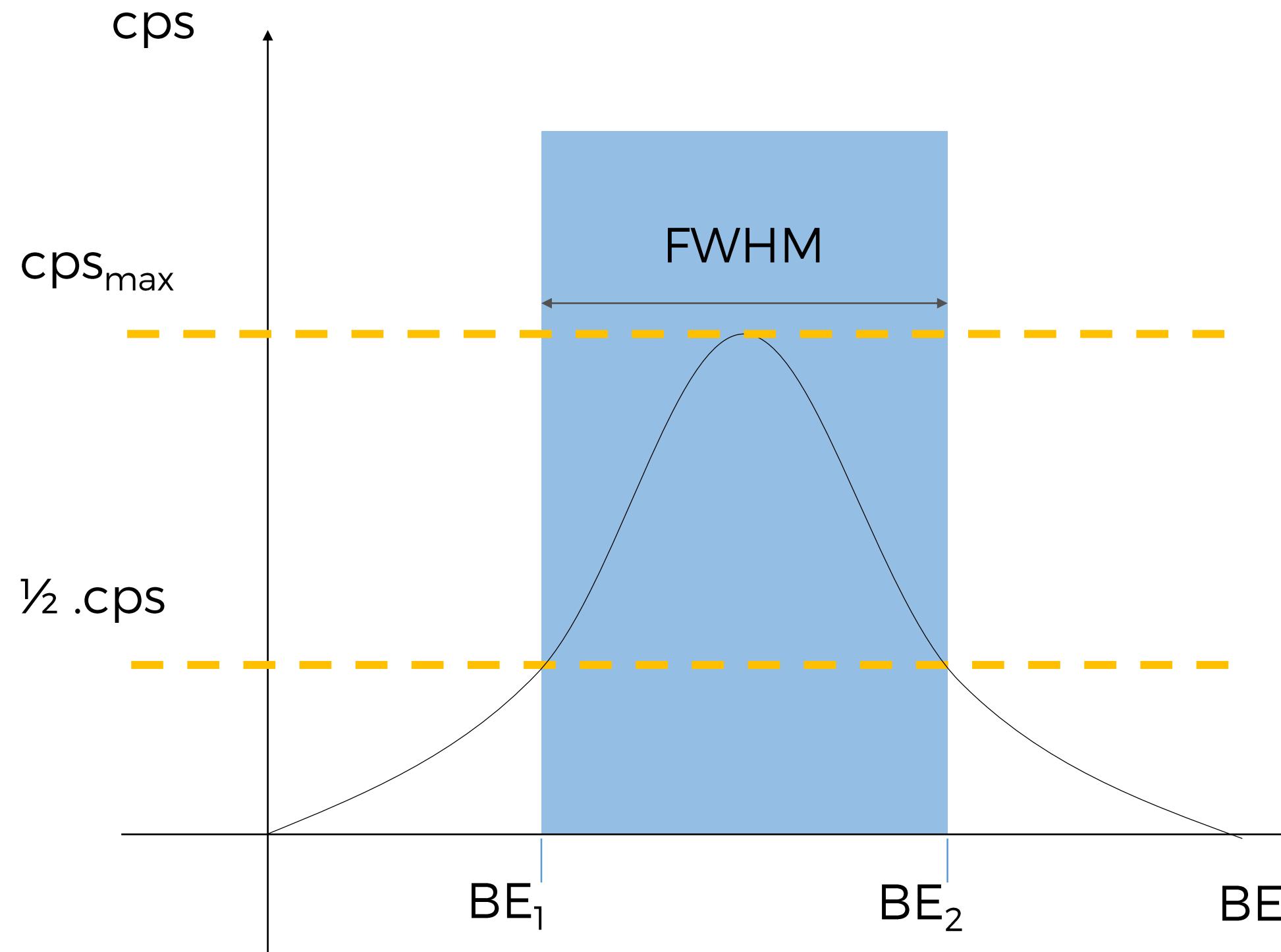


An asymmetric line-shape (Doniach-Sunjic or double Lorentzian) is required when asymmetry is found in the spectra, as for example in pure transition metals.

Double Lorentzian: Lorentzian width is different between the two sides of the peak. Quantification is possible.

Doniach – Sunjic: Theoretically based profile. Not proper for quantification since the functional form is not integrable.

Background
Binding Energy
 Gaussian
 Lorentzian



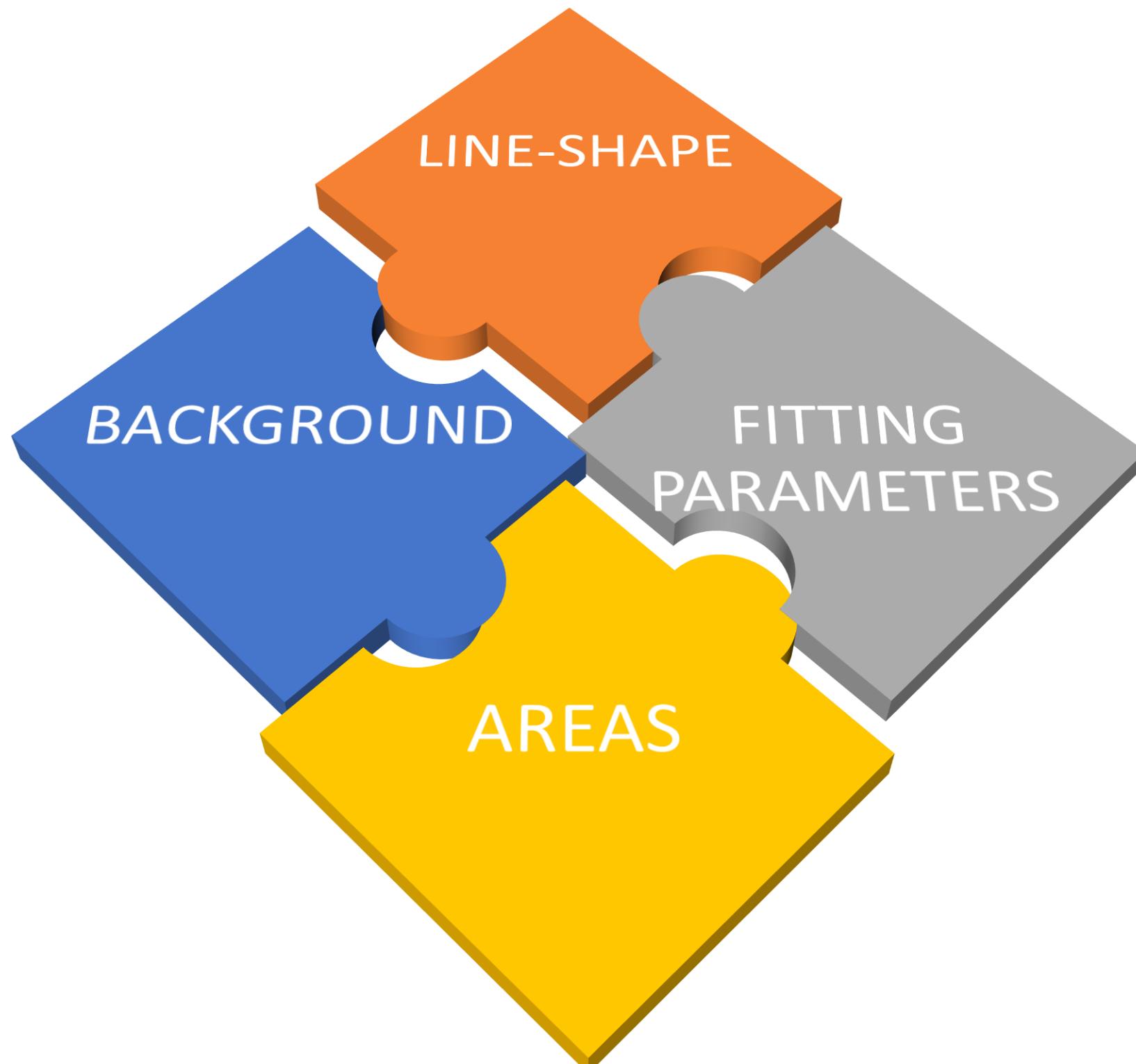
Full width at half height (FWHM) is a mathematical convolution of various contributions:
 natural width of core level, phonon broadening, width of X-ray line, and energy resolution of the analyzer
 Its value can be calculated from Gaussian and Lorentzian values as an approximation to comparison purposes as:

$$FWHM = \sqrt{G^2 + L^2}$$



QUANTITATIVE METHODS

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PHYSICAL PARAMETERS (first principles)

(Assuming a homogeneous sample)

$$N_A = \frac{I_A KE}{\frac{d\sigma}{d\Omega} \lambda}$$

$$\frac{d\sigma}{d\Omega} = \frac{\sigma}{4\pi} \left[1 + \beta_2^1 \left(3 \sin^2 \alpha \frac{\cos^2 2\chi}{1 + \cos^2 2\chi} - 1 \right) \right]$$

N_A = density of atoms [atoms/cm²]

I_A = Detector count rate [(electrons/volume)(volume)]

KE = Kinetic energy of the emitted photoelectron

$\frac{d\sigma}{d\Omega}$ = photoelectric scattering cross section [cm²]

λ = electron attenuation length [cm]

β = asymmetry parameter

α = angle between the x ray source and the detector axis

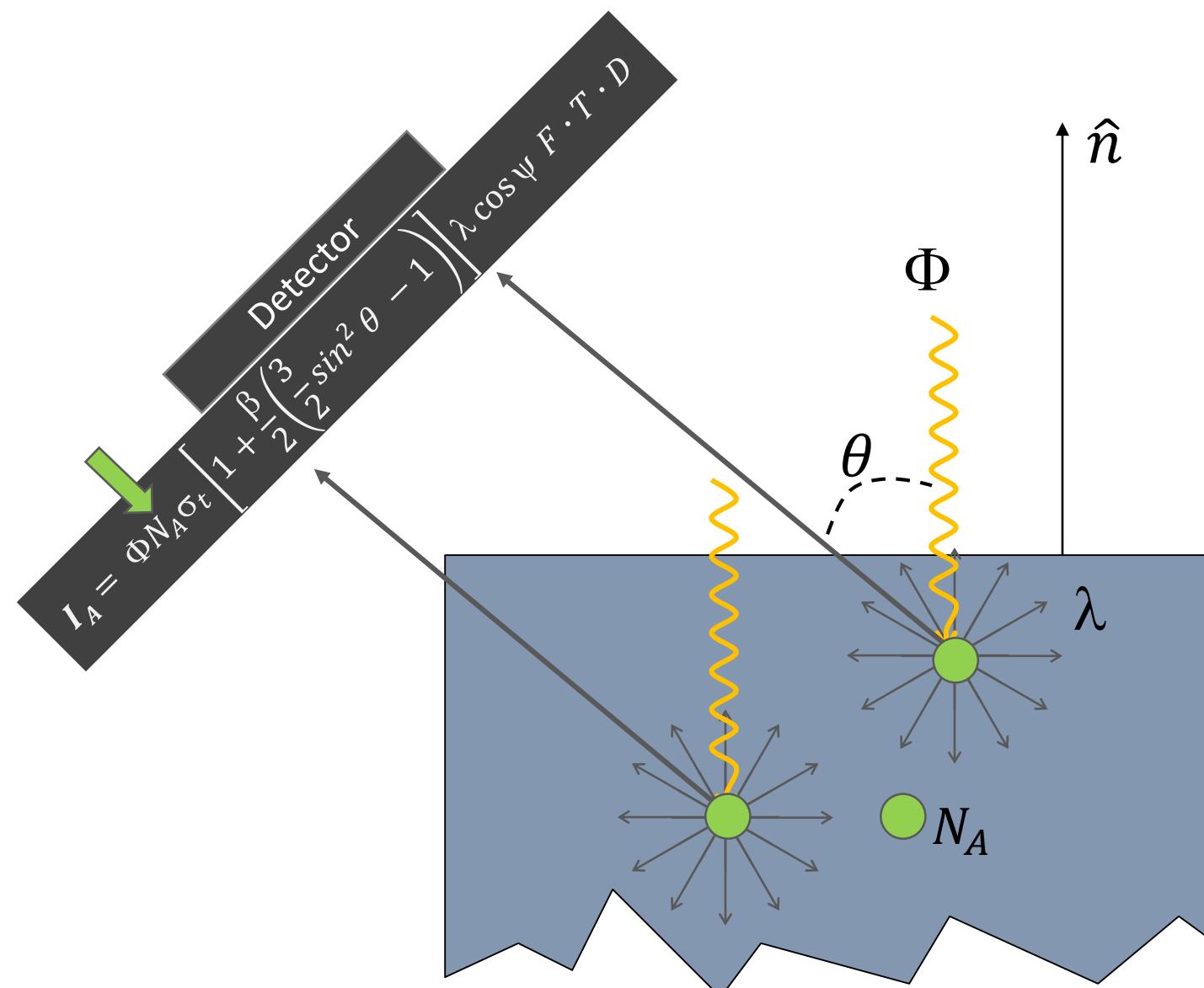
χ = angle between the incident beam and the reflected on the monochromator



QUANTITATIVE METHODS

63

PHYSICAL PARAMETERS



$$R_A^{a\%} = \frac{N_A}{\sum_j N_B} \cdot 100$$

PHYSICAL PARAMETERS (first principles)

(Assuming a homogeneous sample)

$$N_A = \frac{I_A KE}{\frac{d\sigma}{d\Omega} \lambda}$$

$$\frac{d\sigma}{d\Omega} = \frac{\sigma}{4\pi} \left[1 + \beta_2^1 \left(3 \sin^2 \alpha \frac{\cos^2 2\chi}{1 + \cos^2 2\chi} - 1 \right) \right]$$

N_A = density of atoms [atoms/cm²]

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α = angle between the x ray source and the detector axis

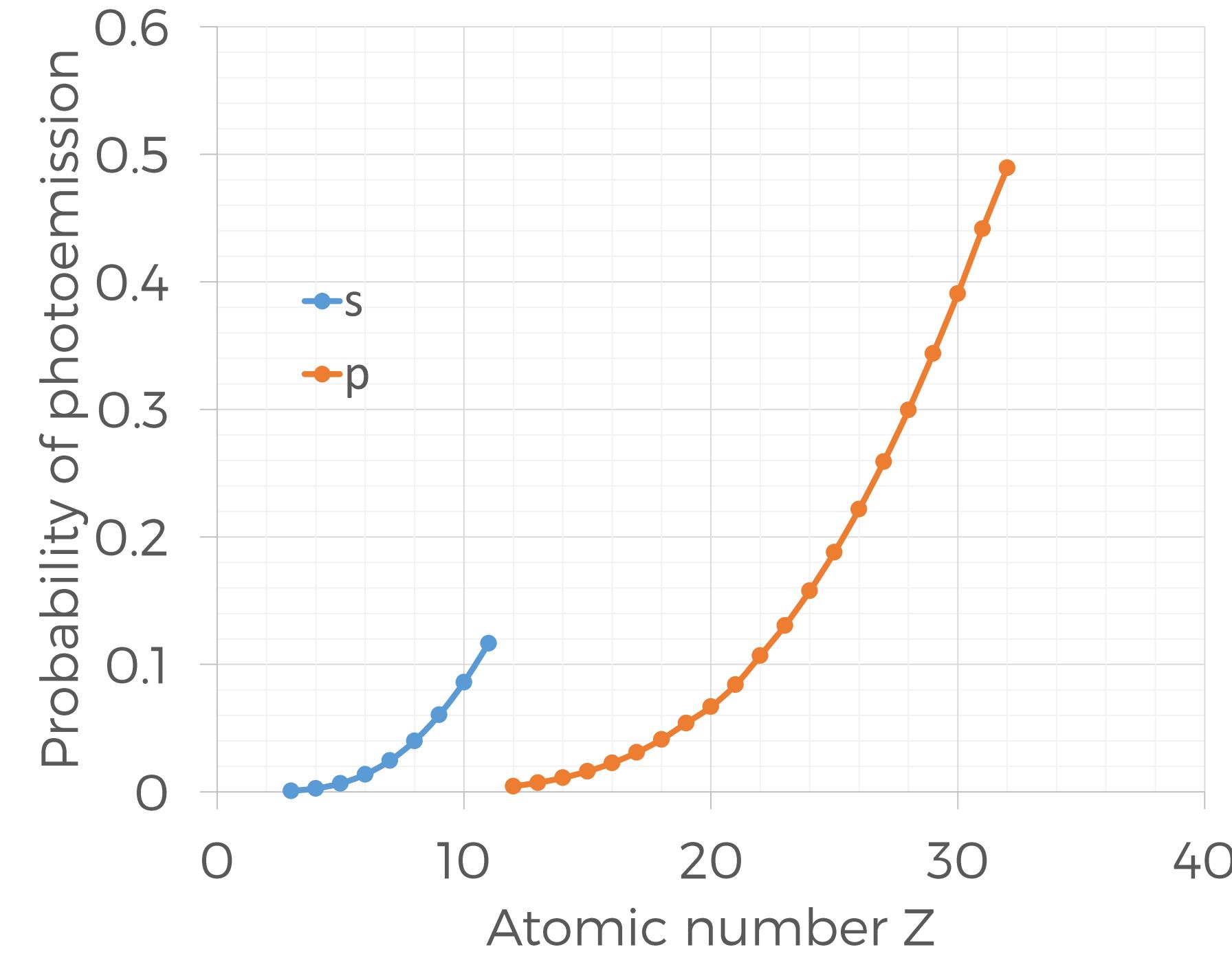
χ = angle between the incident beam and the reflected on the monochromator



QUANTITATIVE METHODS

64

CROSS SECTION



The cross section is a measure of interaction between photons and scattered atoms present in a material, which has units of area and represents the effective cross section that photons have when approaching the target. This is one of the most important factors in the quantification of spectra obtained by the XPS technique. This is an effective area that gives the number of transitions on average. This is why it is considered as an area that defines a probability of the phenomenon of photoionization occurring.



QUANTITATIVE METHODS

65

NIST Electron Effective-Attenuation-Length Database

Database Input Parameters File Management Comparisons Disclaimer

NIST Standard Reference Database 82

NIST ELECTRON EFFECTIVE-ATTENUATION-LENGTH DATABASE

Version 1.0

Data provided by
C. J. Powell, Surface and Microanalysis Science Division
National Institute of Standards and Technology
Gaithersburg, MD 20899, USA
A. Jablonski, Institute of Physical Chemistry
Polish Academy of Sciences, Warsaw, Poland

Software developed by
A. Jablonski, Institute of Physical Chemistry
Polish Academy of Sciences, Warsaw, Poland

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QUANTITATIVE METHODS

SCOFIELD

QUANTITATIVE METHODS

Battistoni, C., Mattogno, G. and Paparazzo, E.

QUANTITATIVE SURFACE ANALYSIS BY XPS: A COMPARISON AMONG DIFFERENT QUANTITATIVE APPROACHES

Atomic ratio determinations in a series of pure inorganic compounds have been derived from XPS peak intensity measurements taken by area via the so-called 'first principles model' (FPM) and the 'elemental sensitivity factors' (ESF) methods. The two methods show similar degrees of accuracy, with a typical error of about $\pm 10\%$ when a set of experimental ESF is developed.

A lower accuracy, as expected, has been obtained when the literature ESF have been applied. Some discrepancy between the two approaches are evident when the kinetic energy separations of the XPS elemental peaks involved in the atomic ratio calculations is large. This aspect is discussed in the light of instrumental responses which are of primary concern for the transferability of ESF results from one instrument to another.

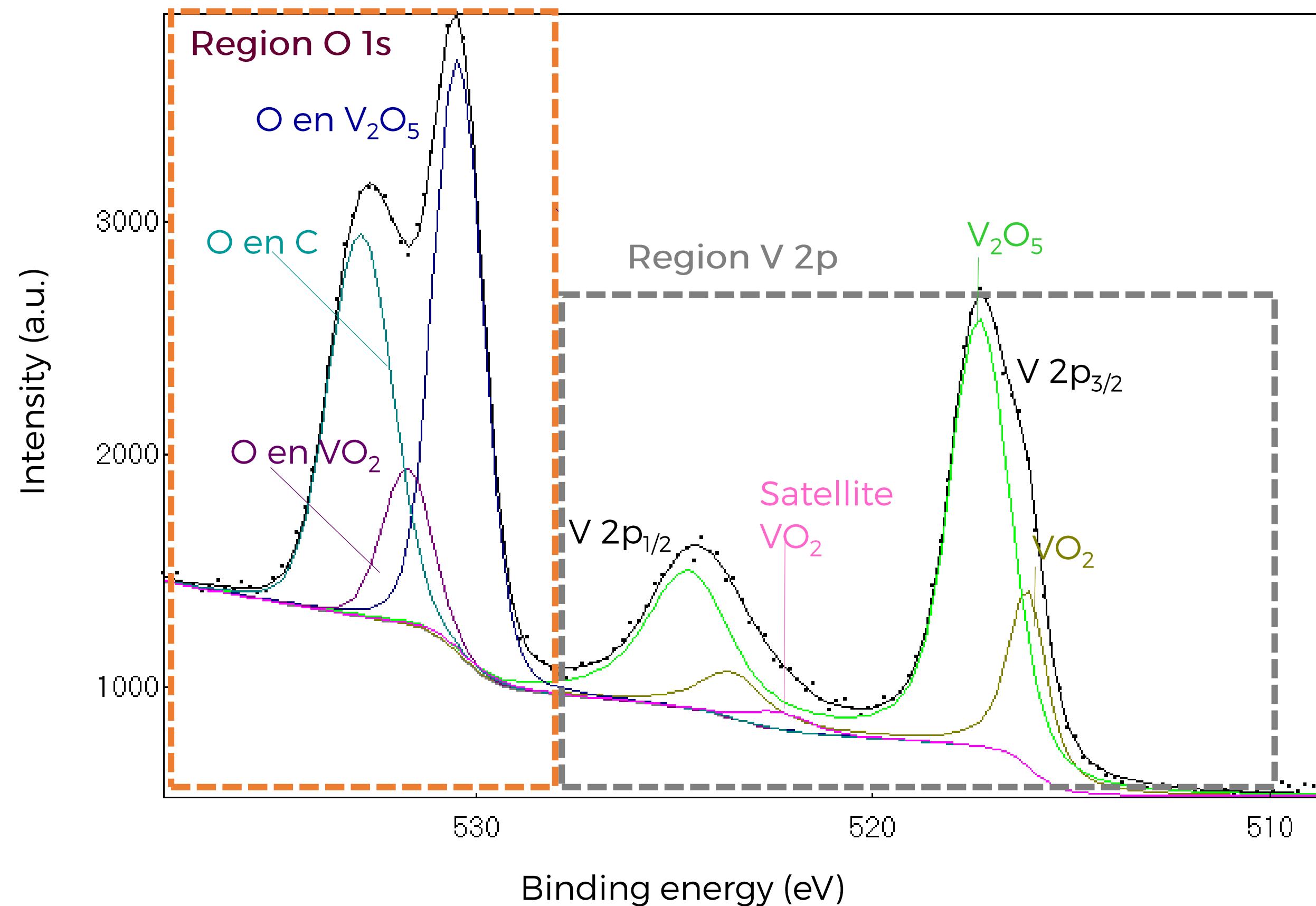
Reprinted with permission from Surf. Interface Anal., 7, 117 (1985), John Wiley and Sons Ltd, Chichester.



QUANTITATIVE METHODS

QUANTIFICATION

High resolution spectra O 1s and V 2p



$$N_i = \frac{(\text{Area}_i * \text{Kinetic Energy}_i)}{(\sigma_i * I_i)}$$

$$R_A^{ar} = \frac{N_A}{N_B} \cdot n_B$$

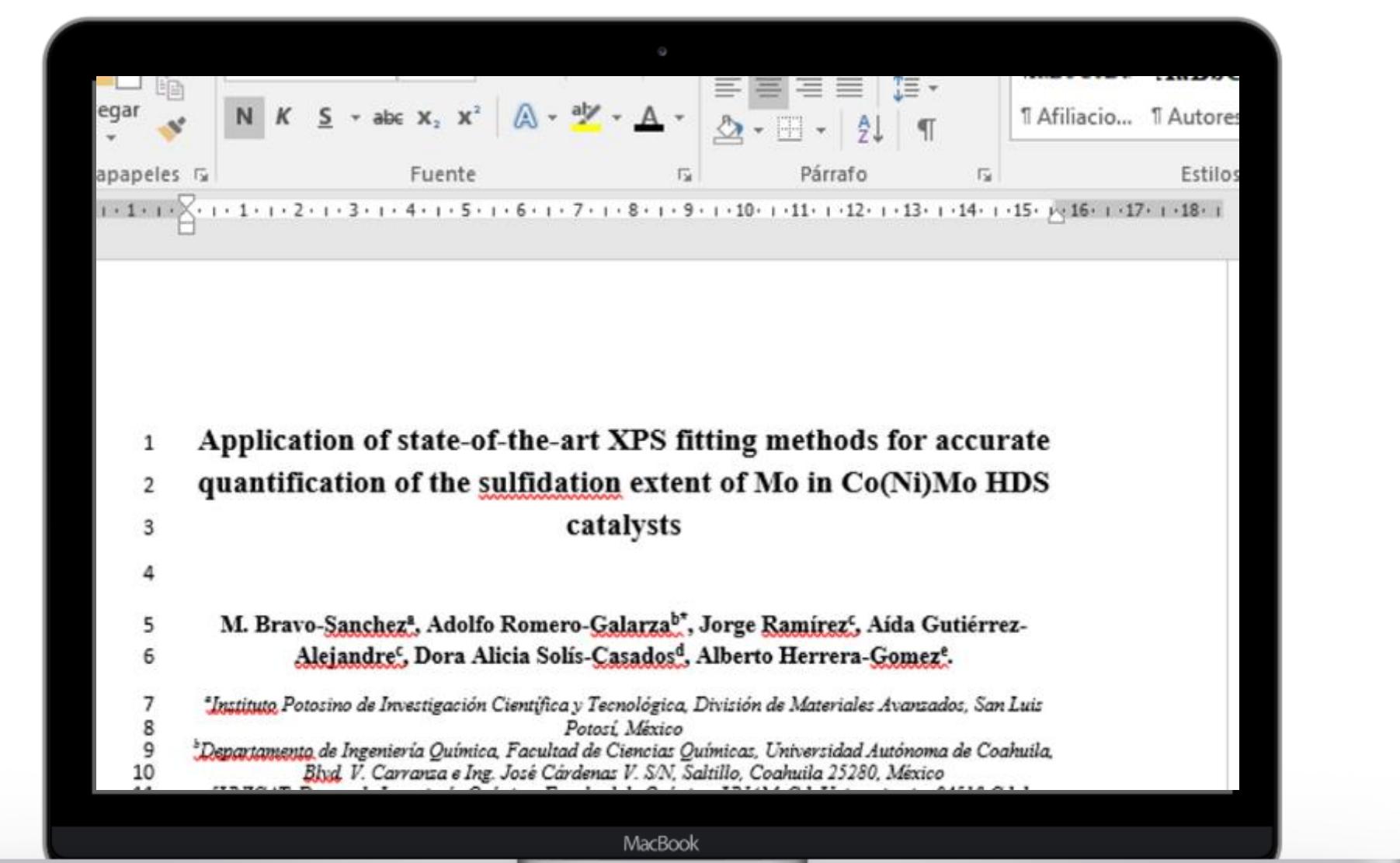
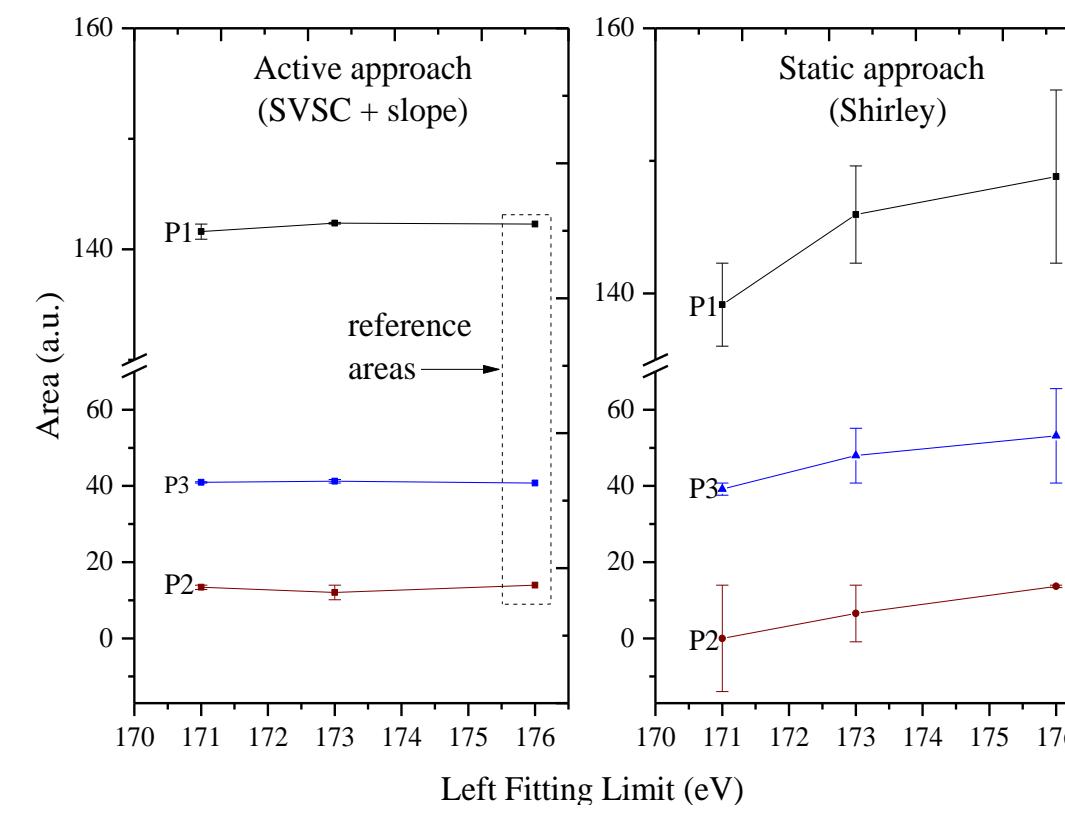
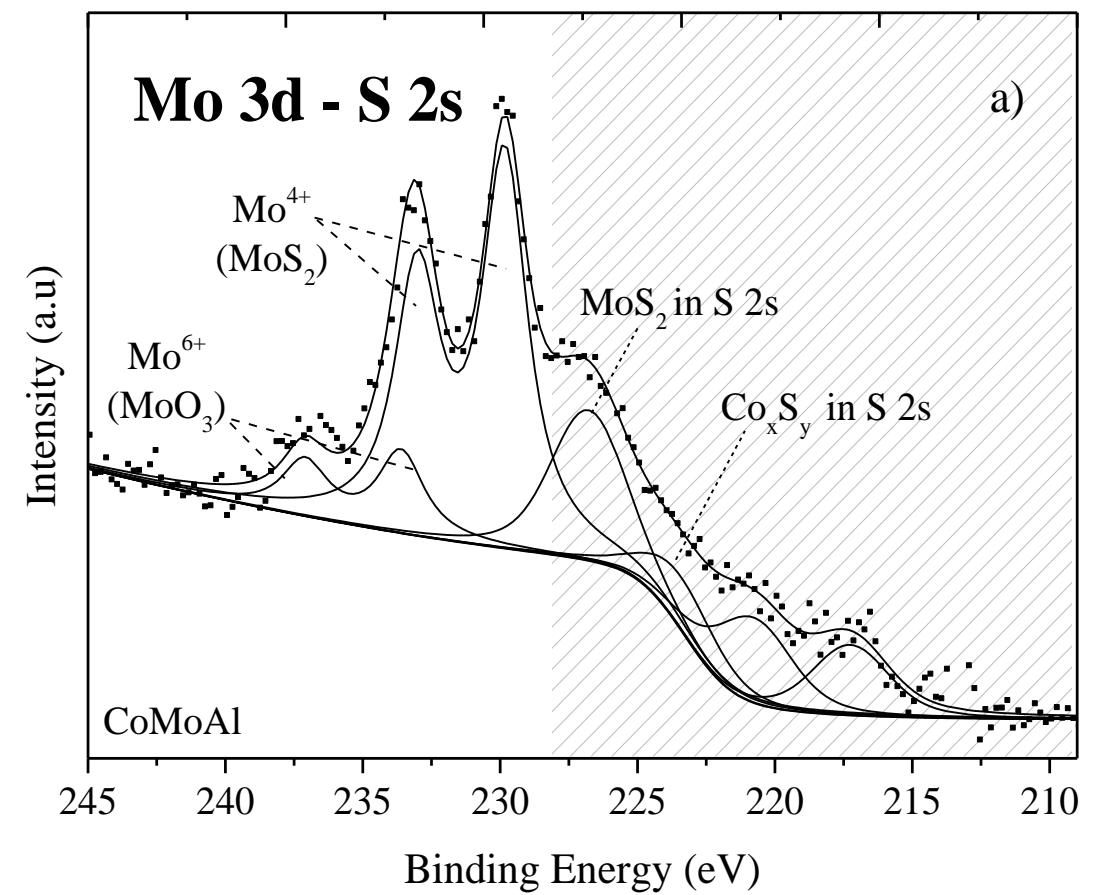
Where N_B and n_B are the concentration and the number of atoms of a particular element and the selected base element, respectively.

Define empirical formula

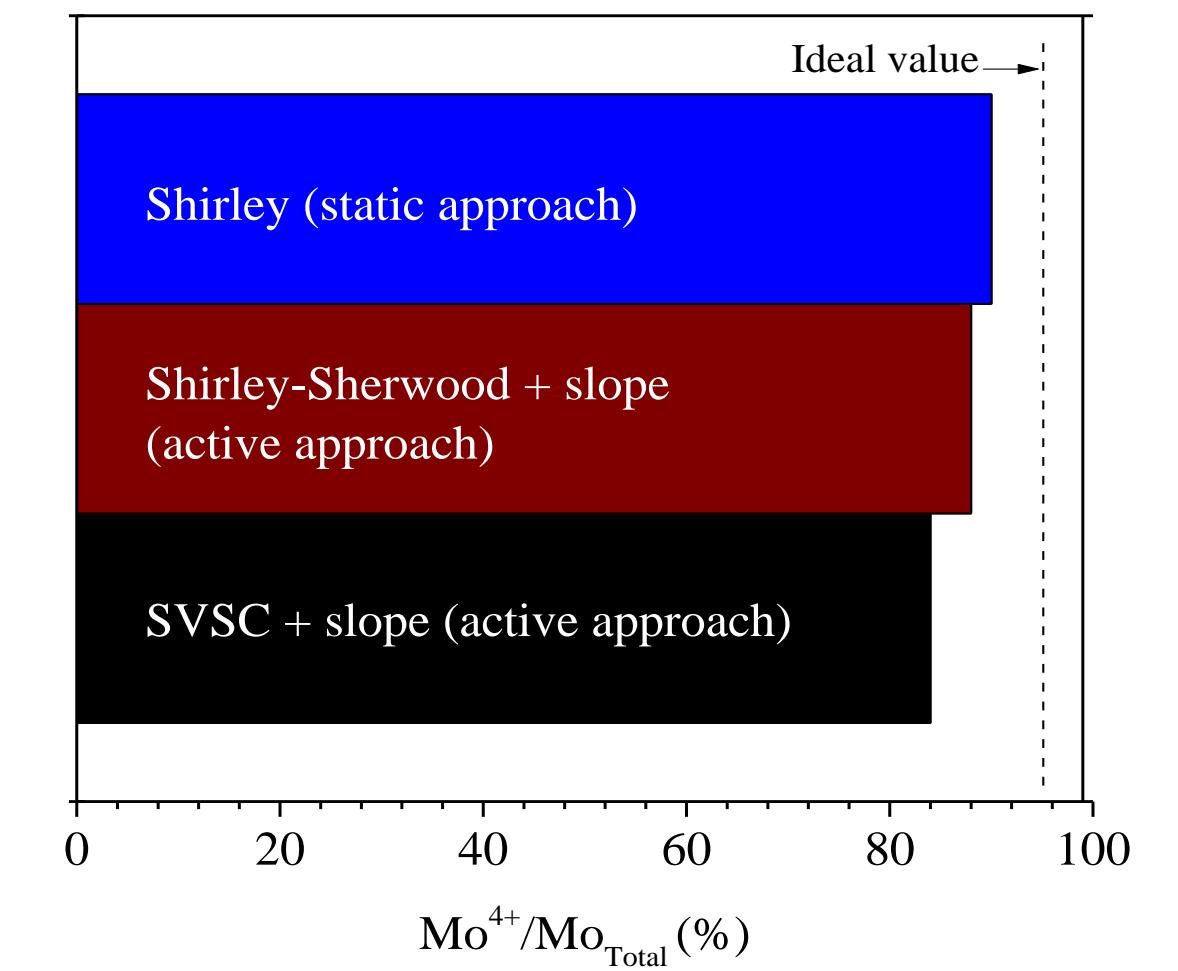
Element	Stoichiometry	
O 1s	2	5
V 2p	0,56	1,85

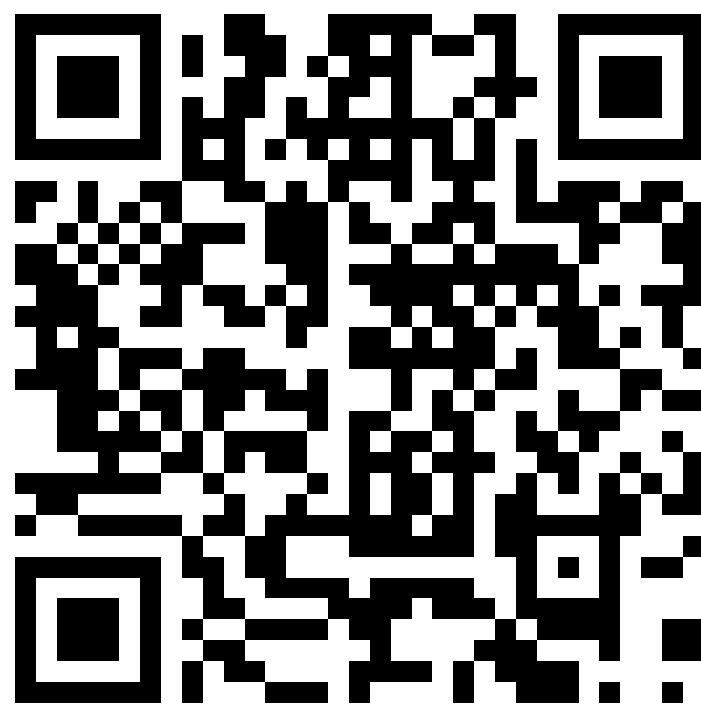
CATALYSIS

About the application of novel empirical methods for obtaining sulfidation extent of Mo in CoMo and NiMo HDS catalyst*



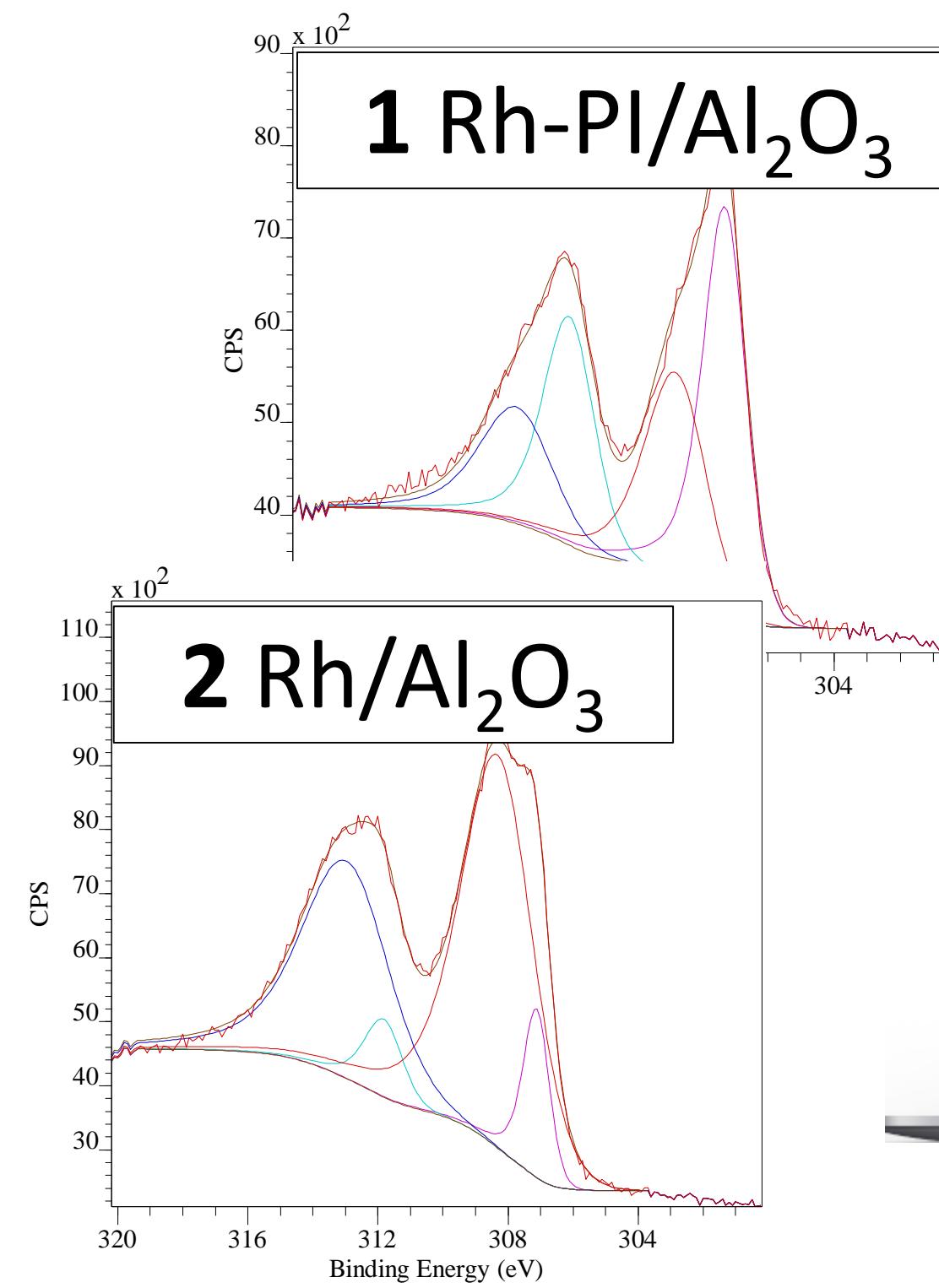
Mo⁴⁺/Mo_{Total}





CATALYSIS

Highlight differences in catalyst surface composition or oxidation state of Rh
that could explain the trend*



Catalysis Science & Technology

PAPER

Check for updates

Cite this: DOI: 10.1039/c7cy01006k

Water as a catalytic switch in the oxidation of aryl alcohols by polymer incarcerated rhodium nanoparticles†

Jack O. Weston,^a Hiroyuki Miyamura,^b Tomohiro Yasukawa,^b Dedi Sutarma,^a Chloe A. Baker,^a Preabjot K. Singh,^a Mariela Bravo-Sanchez,^c Naoko Sano,^c Peter J. Cumpson,^c Yulia Ryabenkova,^d Shū Kobayashi,^b and Marco Conte ^{b,a}

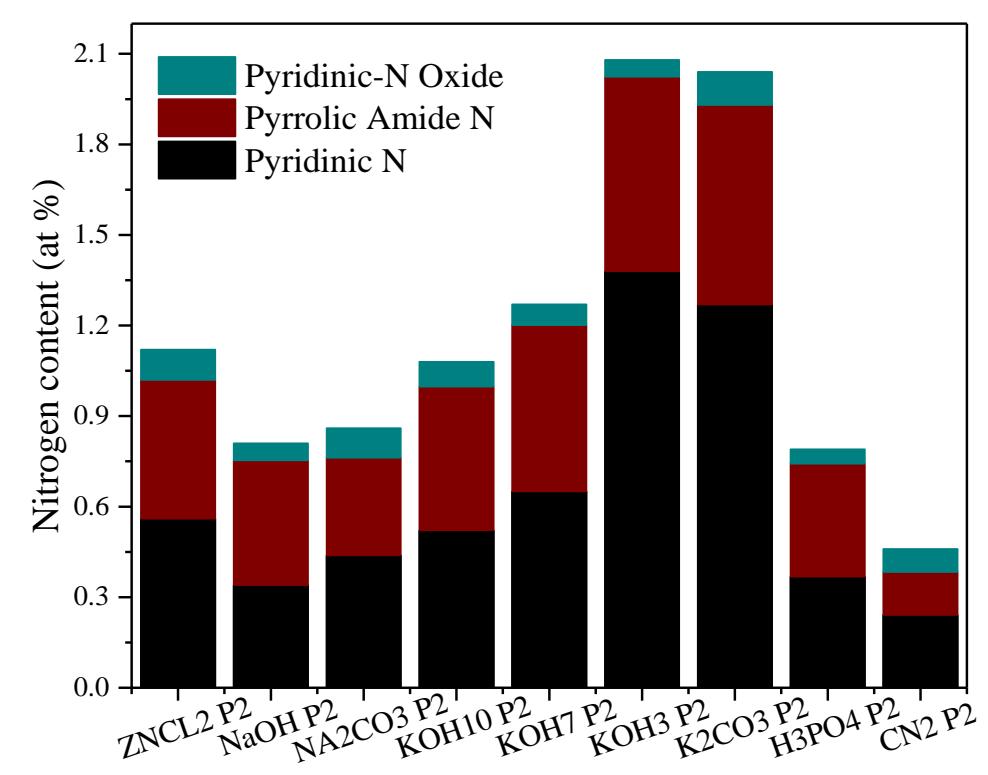
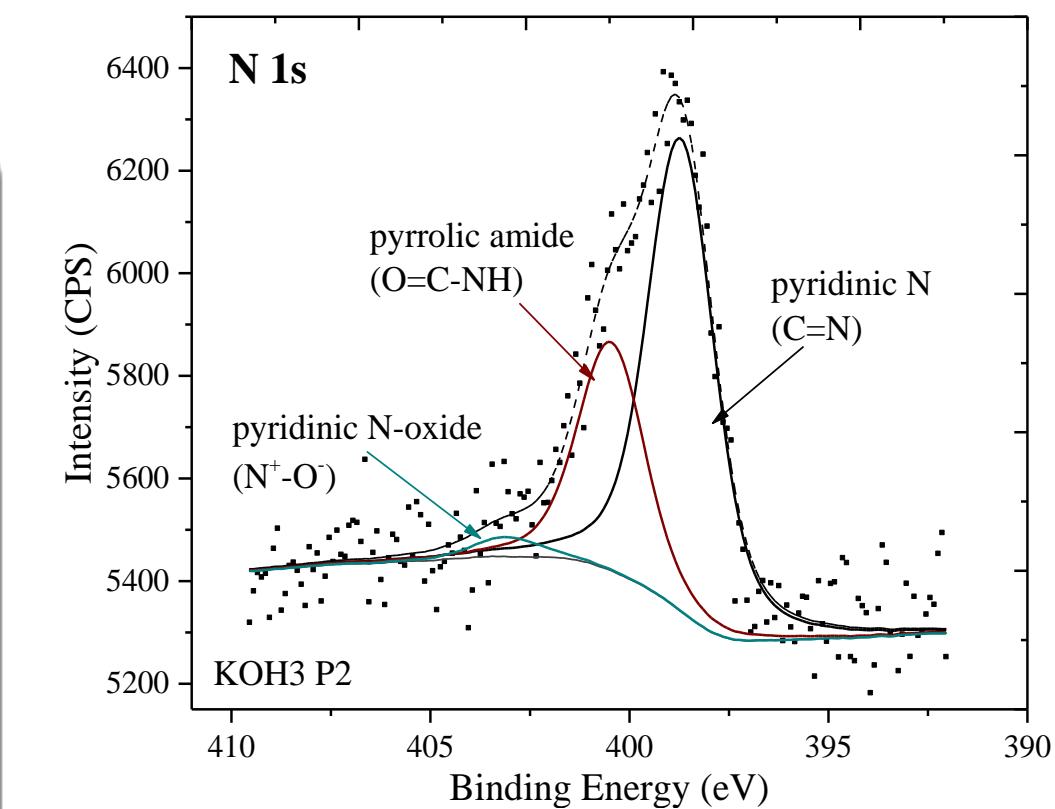
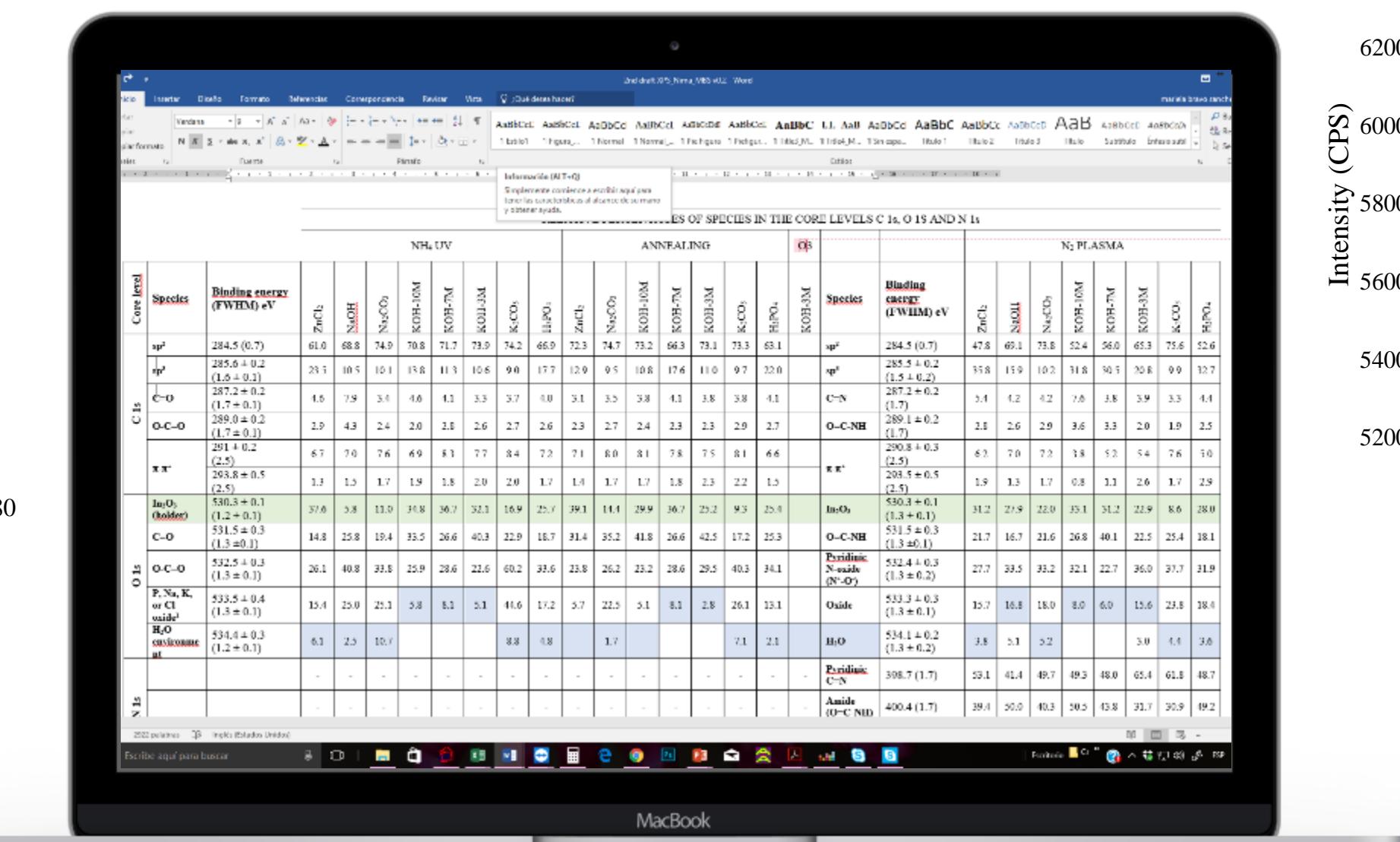
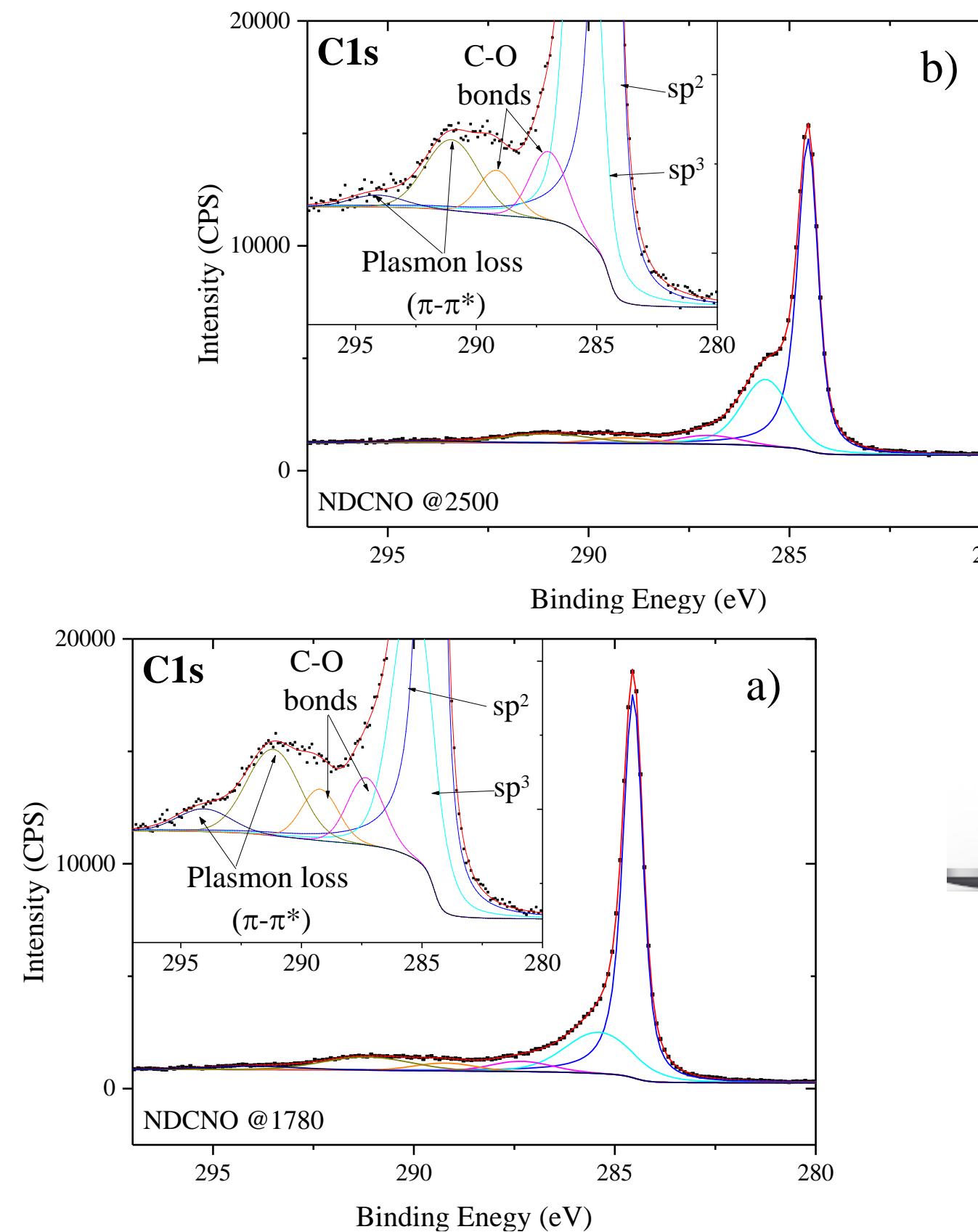
One of the major goals in the oxidation of organic substrates, and especially for alcohol oxidation, is the use of molecular oxygen as the oxidant under mild conditions. Here we report the synthesis and testing of Rh polymer incarcerated catalysts, using a metal so far not used for alcohol oxidation reactions, in which the catalytic activity towards aryl alcohol oxidation, for substrates like 1-phenylethanol and benzyl alcohol, is switched on by the addition of water as co-solvent in toluene. This is done by using air as oxidant at atmospheric pressure, in one of the mildest reaction conditions reported for this class of reaction. The promoting effect of water to higher conversions was observed also for rhodium over alumina supported cata-

Rh₂O₃
1 - 46%
2 - 65%

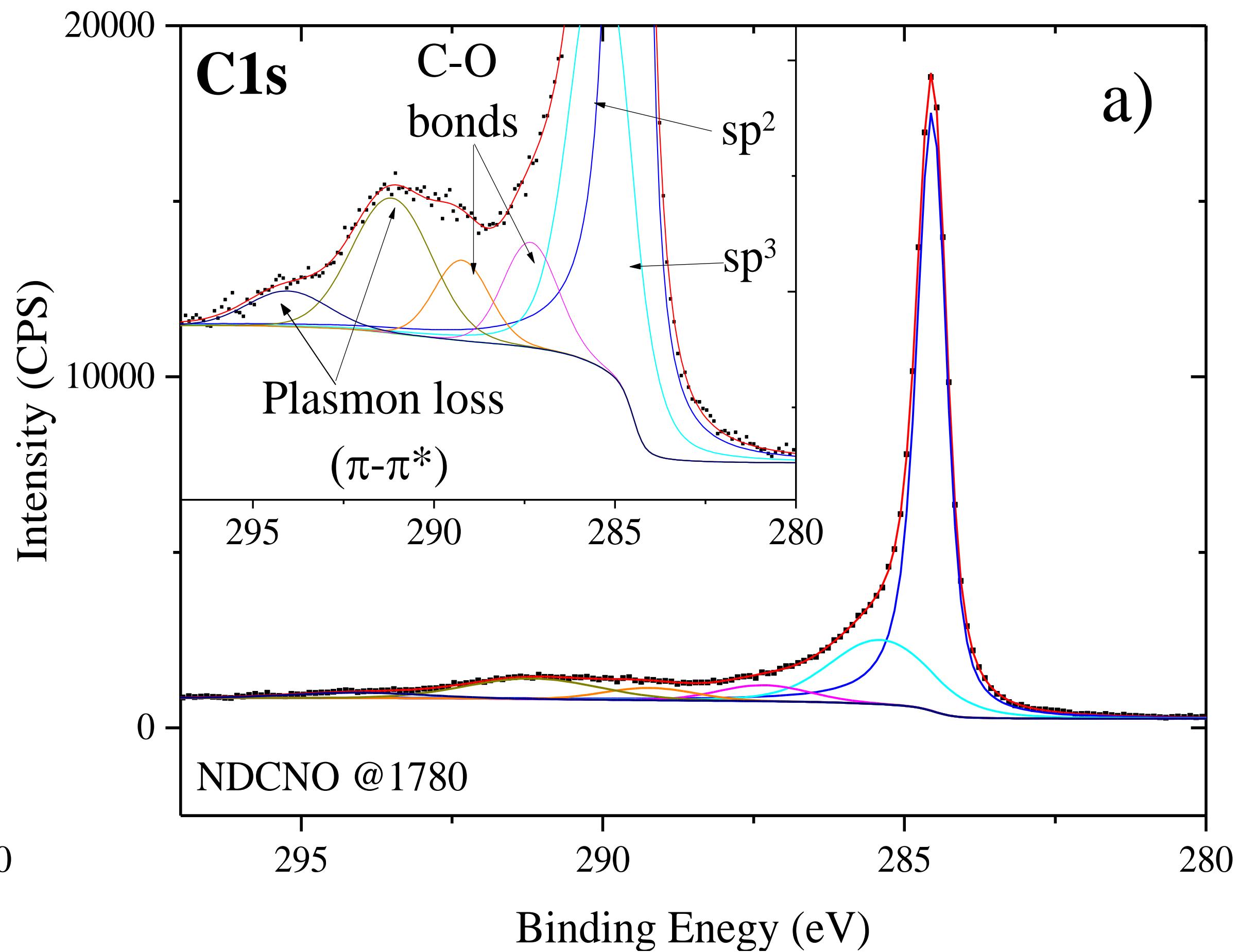
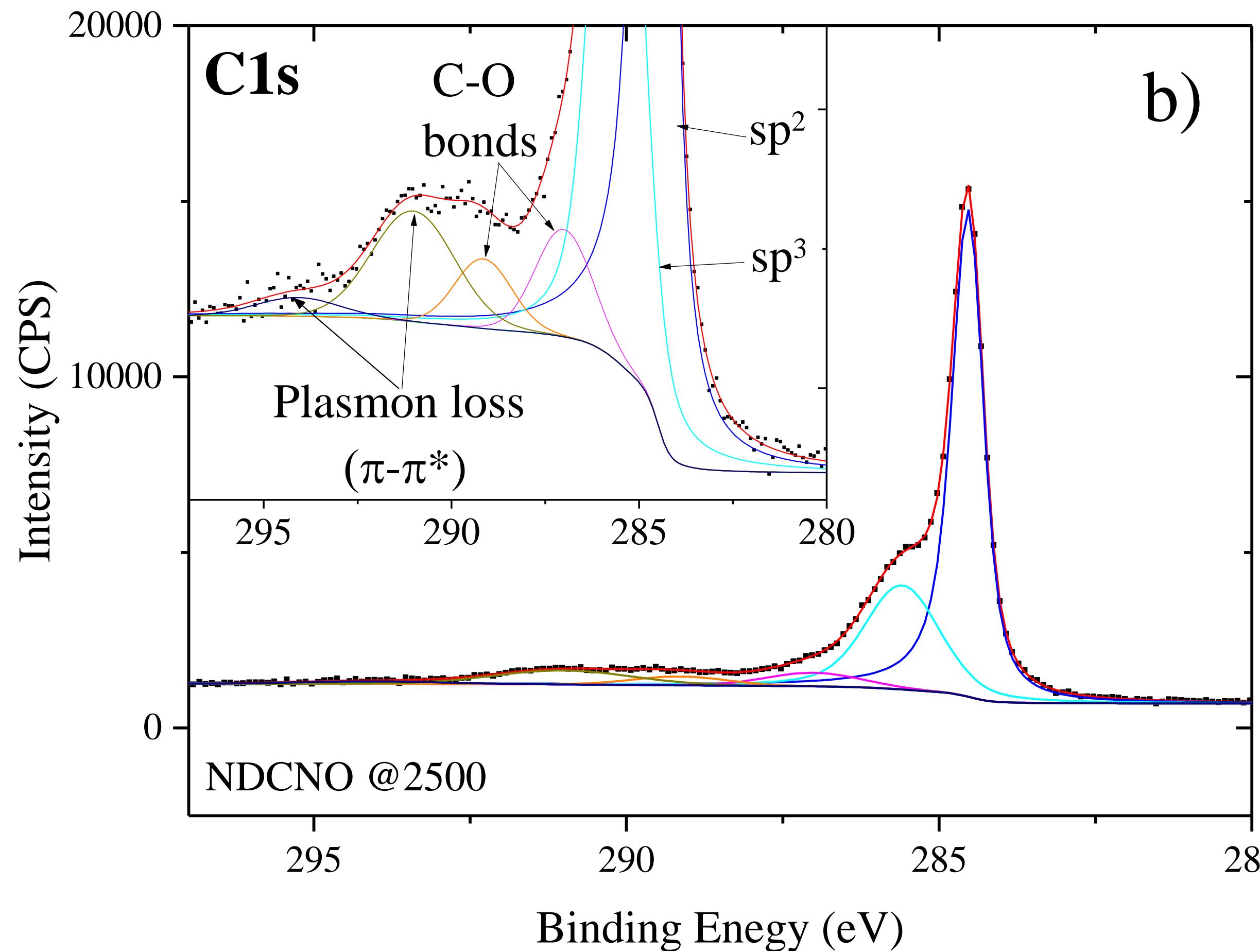


CARBON NANOSTRUCTURES

Evaluation of effectivity of methods for the conversion of nano-diamonds to carbon nano-onions and the after functionalization with physical and chemical methods*



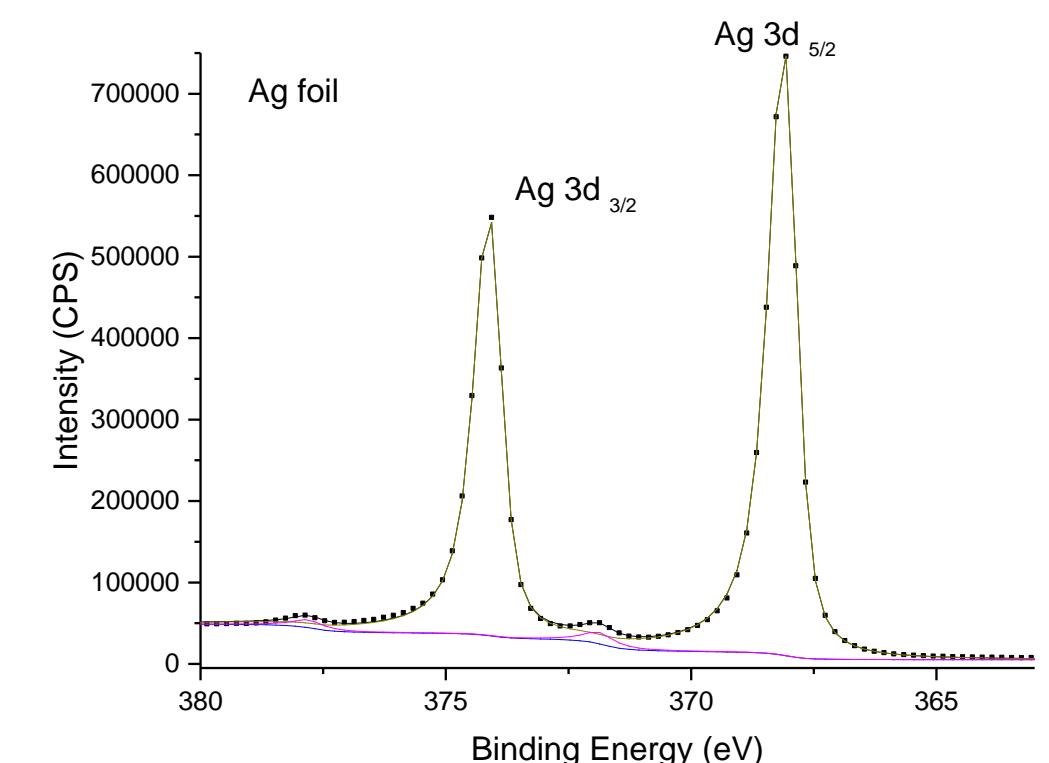
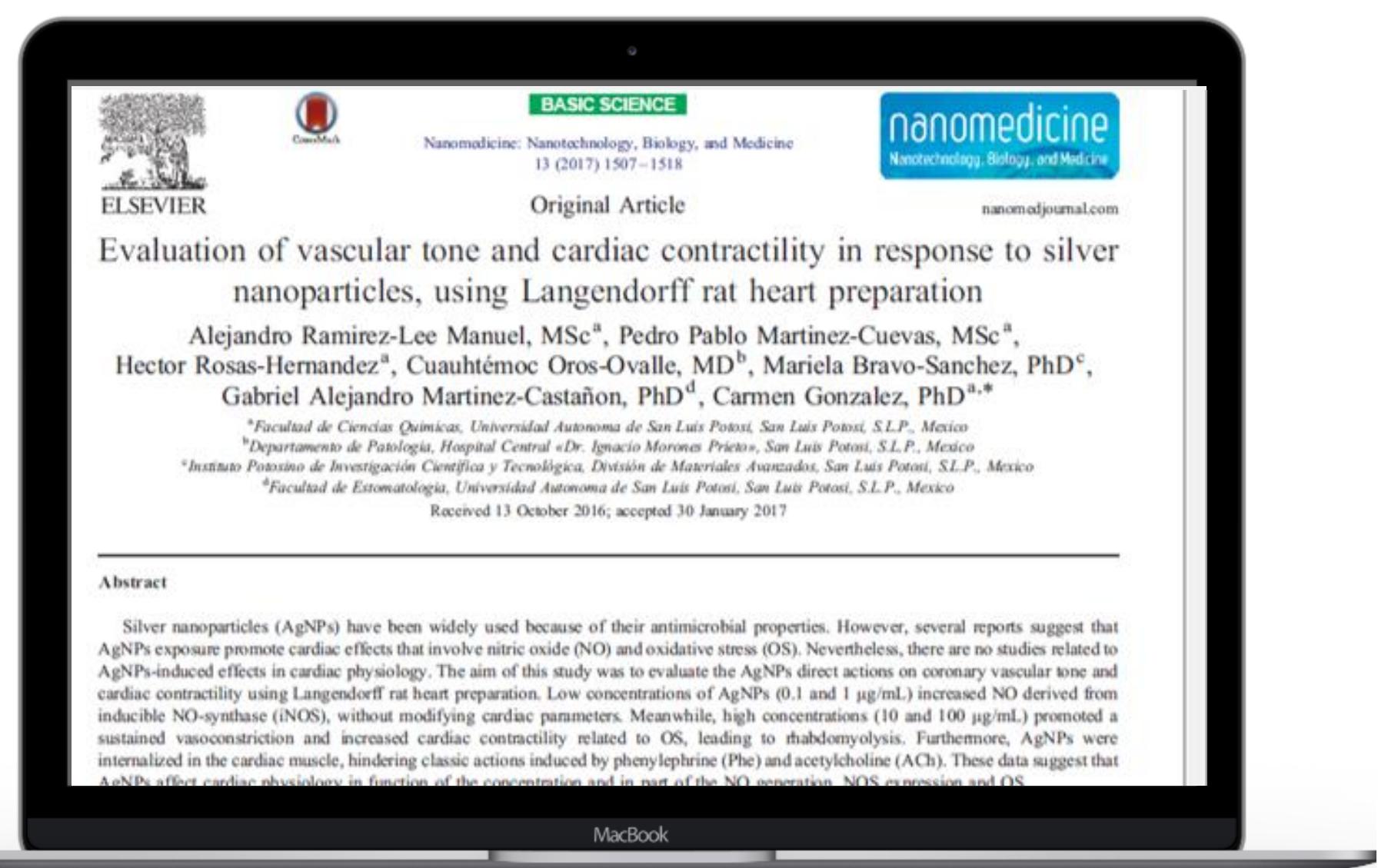
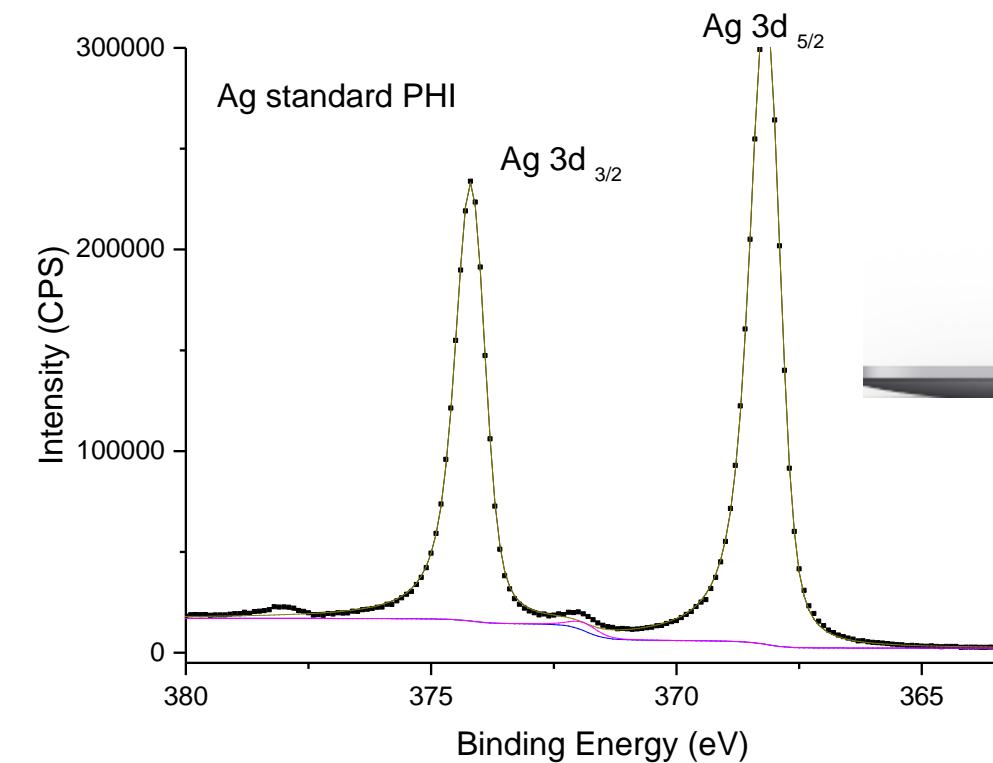
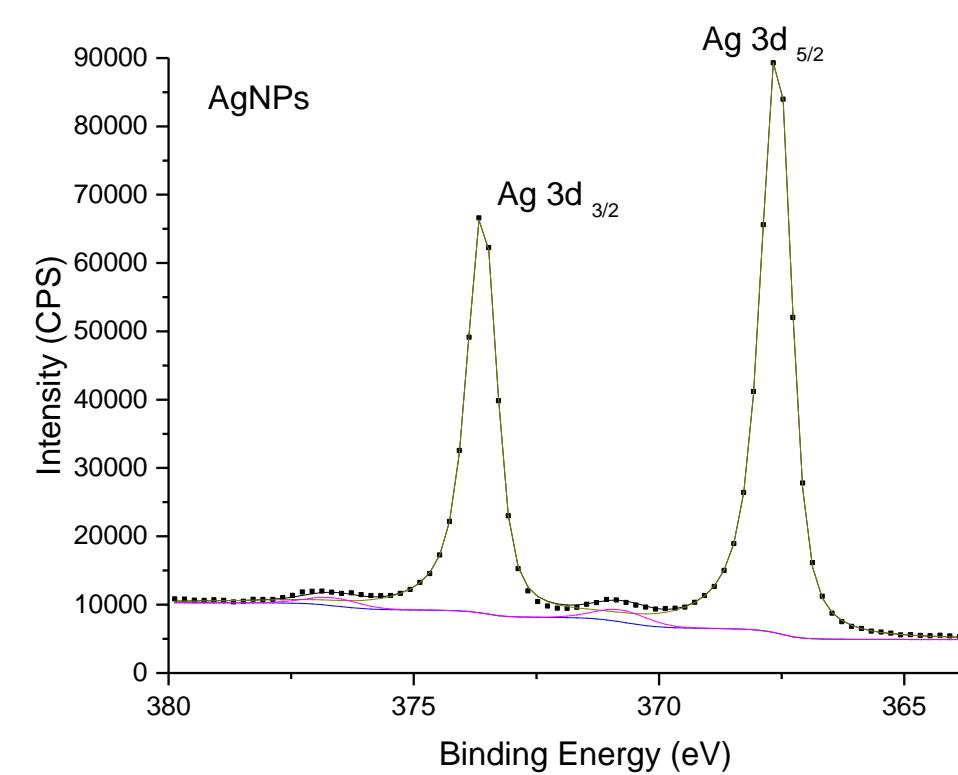
Evaluation of effectivity of methods for the conversion of nano-diamonds to carbon nano-onions





NANOMEDICINE

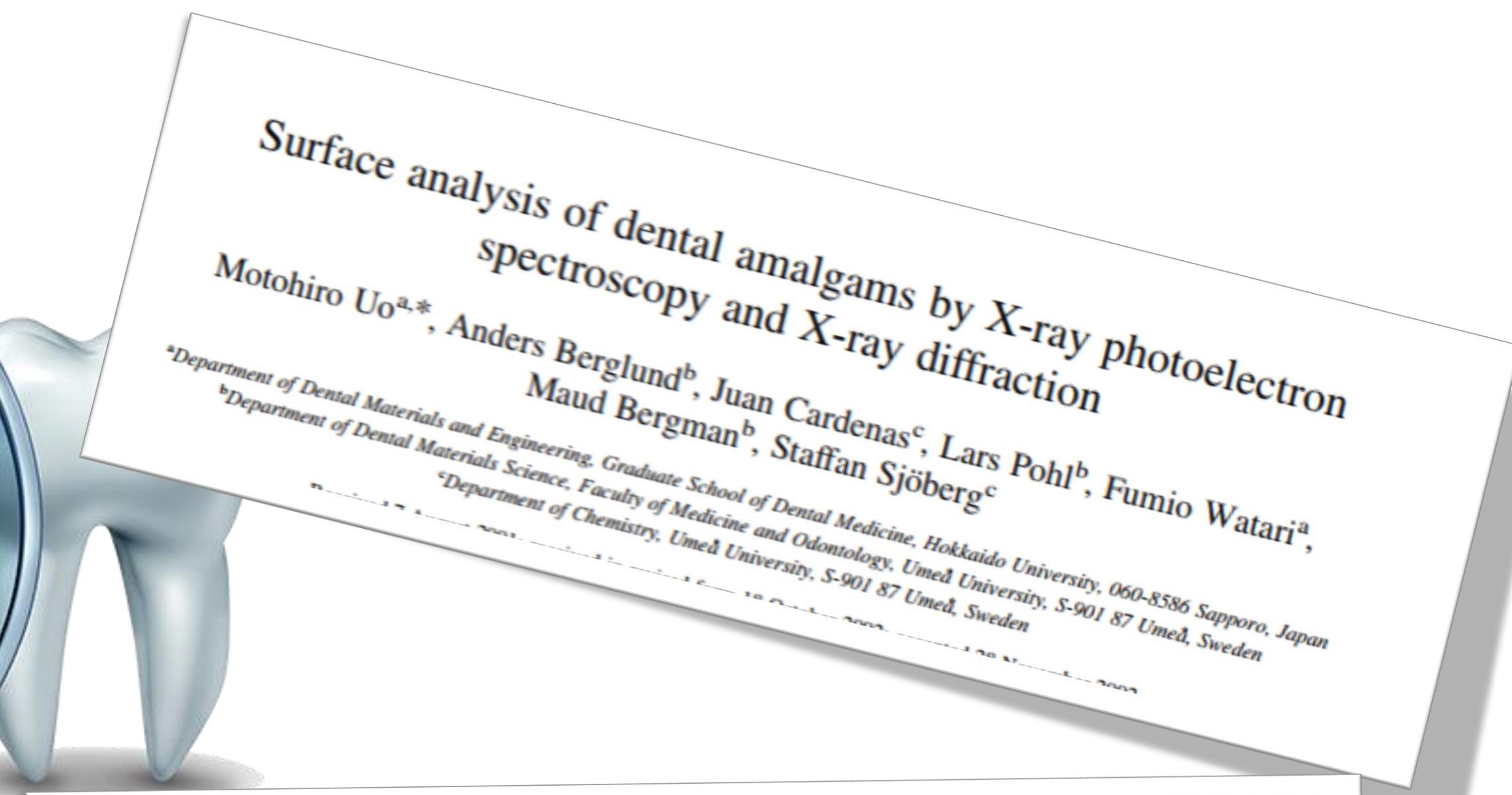
Confirmation of purity of the silver nanoparticles synthetized wit gallic acid for its use in the response evaluation of vascular tone and cardiac contractility*.



FWHM
 0.73 ± 0.02 eV



XPS IN ODONTOLOGY?



Chemical analyses in dental adhesive technology

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ORIGINAL RESEARCH

Biomechanical evaluation and surface characterization of a nano-modified surface on PEEK implants: a study in the rabbit tibia

Open Access Full Text Article

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 Ryo Jimbo¹
 Per Kjellin²
 Fredrik Currie²
 Bruno Ramos Chrcanovic¹
 Ann Wennerberg¹

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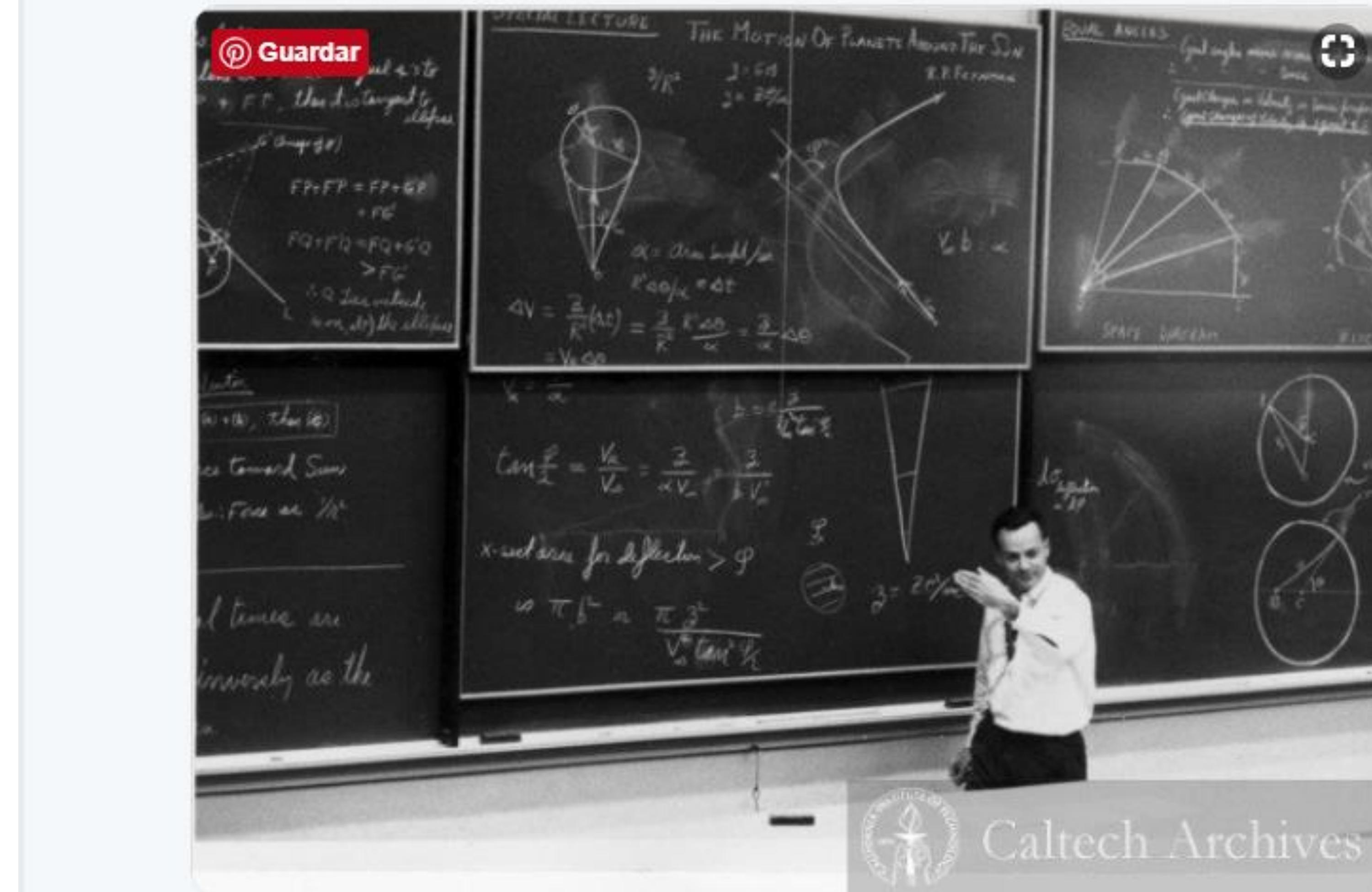
Abstract: Polyether ether ketone (PEEK) is today frequently used as a biomaterial in different medical operations due to its excellent mechanical and chemical properties. However, the untreated surface of PEEK is bioinert and hydrophobic, and it does not osseointegrate in its pure form. The aim of this study was to evaluate a unique nano-modified surface of PEEK with respect to osseointegration. Forty-eight threaded, non-cutting PEEK implants were inserted bilaterally in the tibia of 24 rabbits. Half of the implants ($n=24$) were coated with nanocrystalline hydroxyapatite (test) and the remaining implants ($n=24$) were left uncoated (control). Half of the animals ($n=12$) were euthanized after 3 weeks of healing and the remaining ($n=12$) after 12 weeks. The implant retention was measured with a removal torque apparatus. Surface analysis was performed with interferometry, scanning electron microscopy, and X-ray photon



Richard Feynman @ProfFeynman · Oct 27

I would rather have questions that can't be answered than answers that can't be questioned.

76



16

1.4K

3.5K



Richard Feynman @ProfFeynman · Oct 26

I don't feel frightened by not knowing things.

76

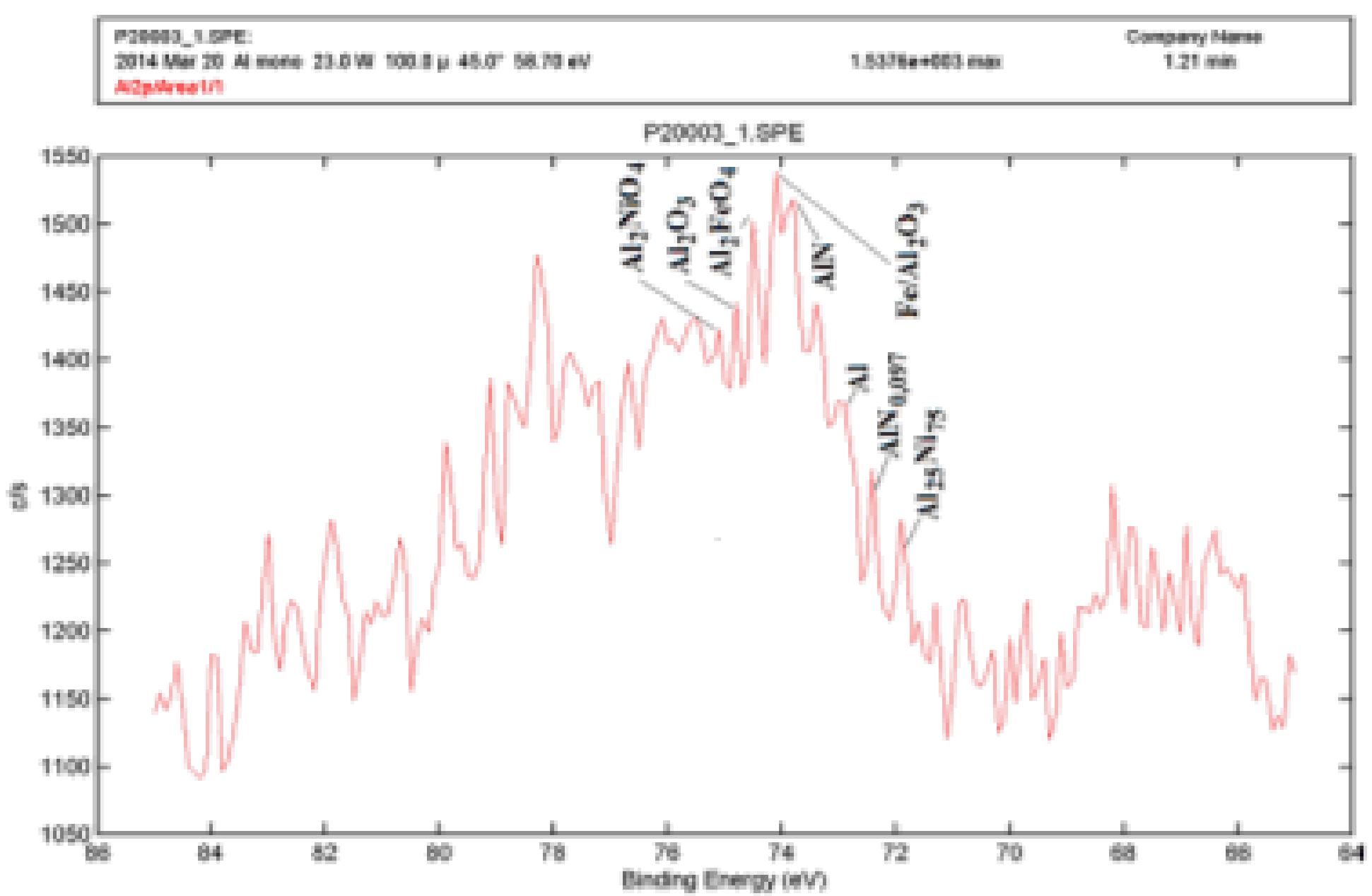
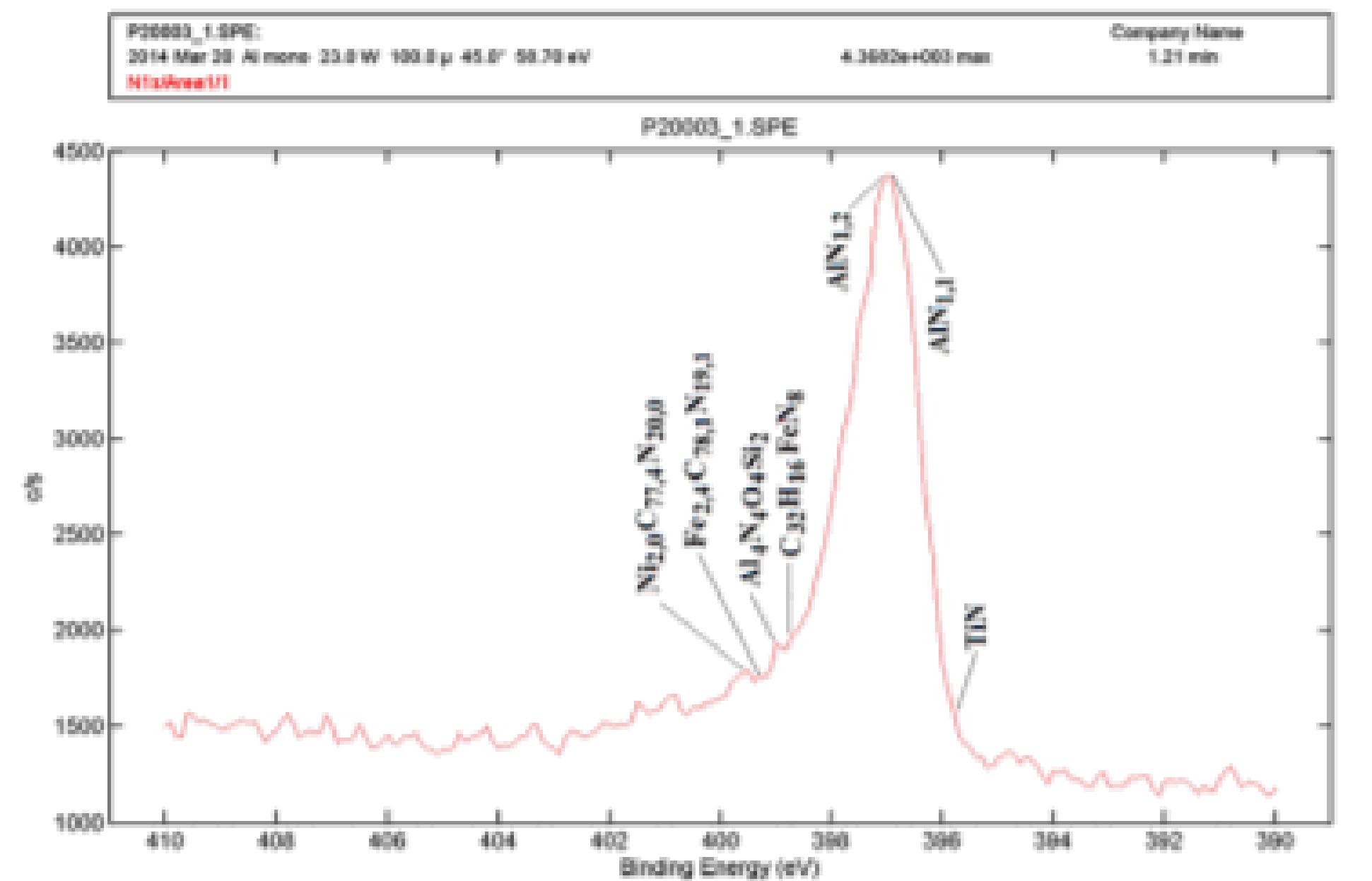
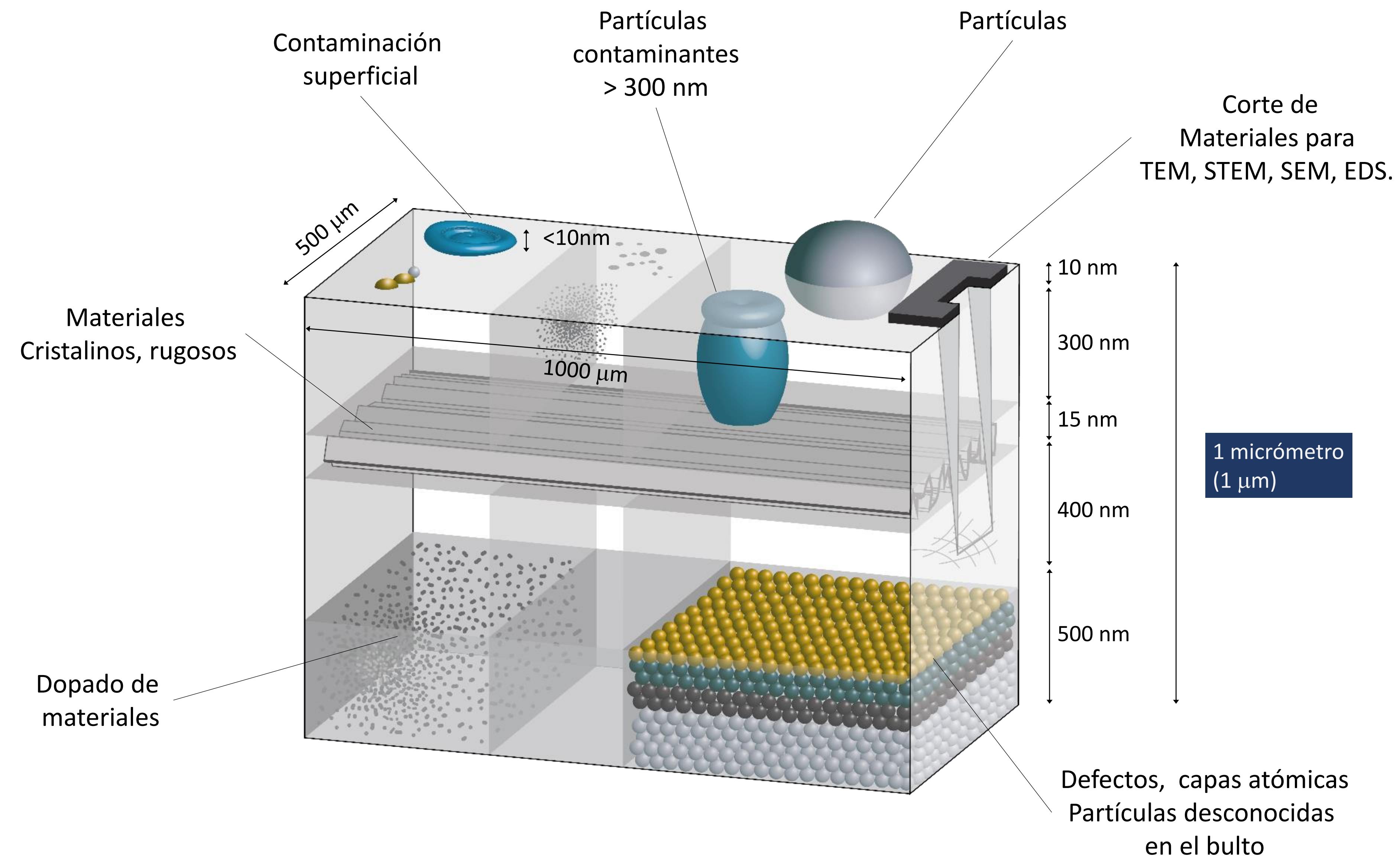
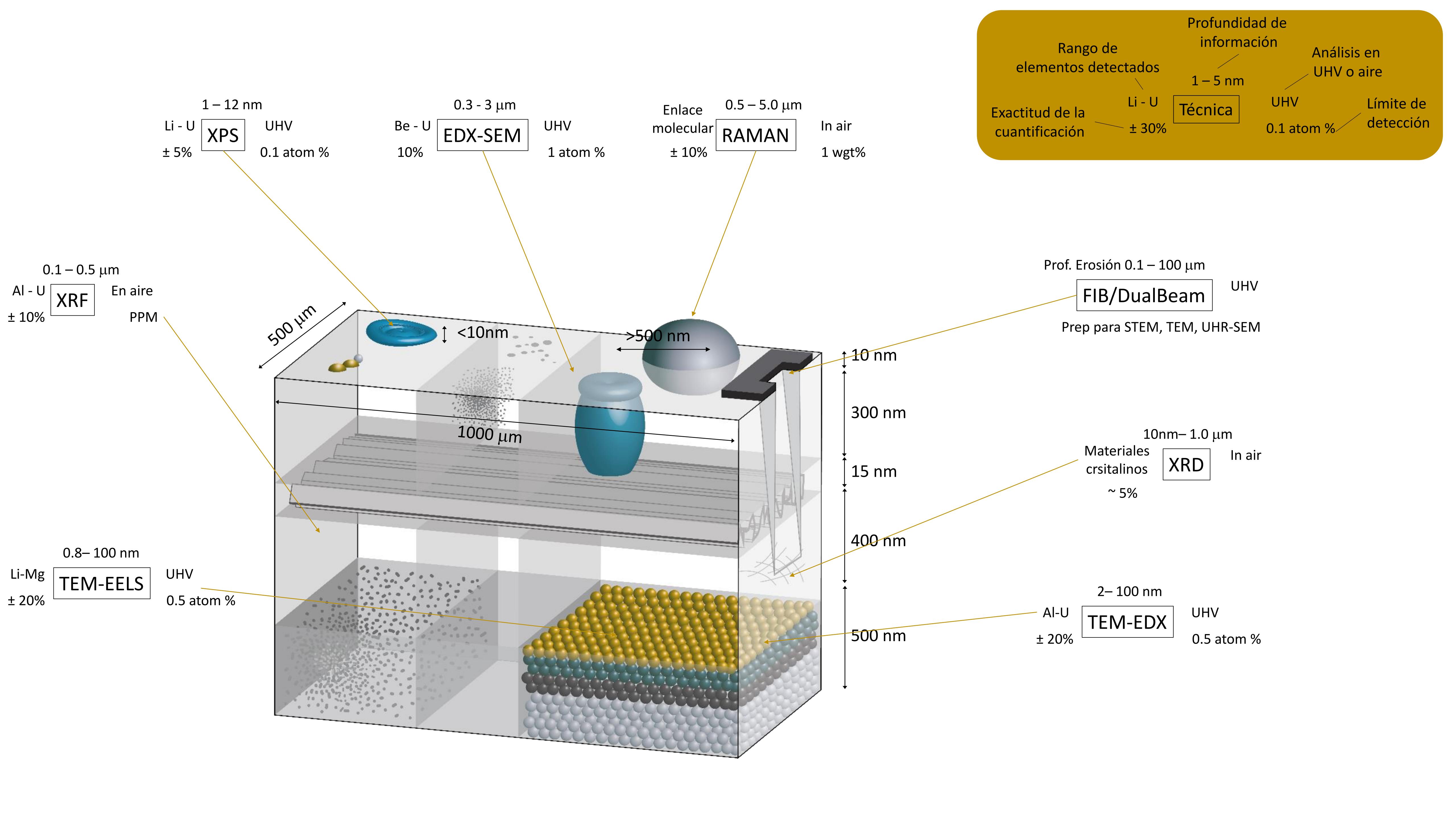


Figure 9. XPS analysis for Al2p for stainless steel sample $R_s = 3.2 \mu\text{m}$, highlighted peaks for following chemical compounds: ($\text{Al}_{25}\text{Ni}_{75}$, $\text{AlN}_{0.097}$, AlN , $\text{Fe}/\text{Al}_2\text{O}_3$, Al_2FeO_4 , Al_2O_3 , Al_2NiO_4).





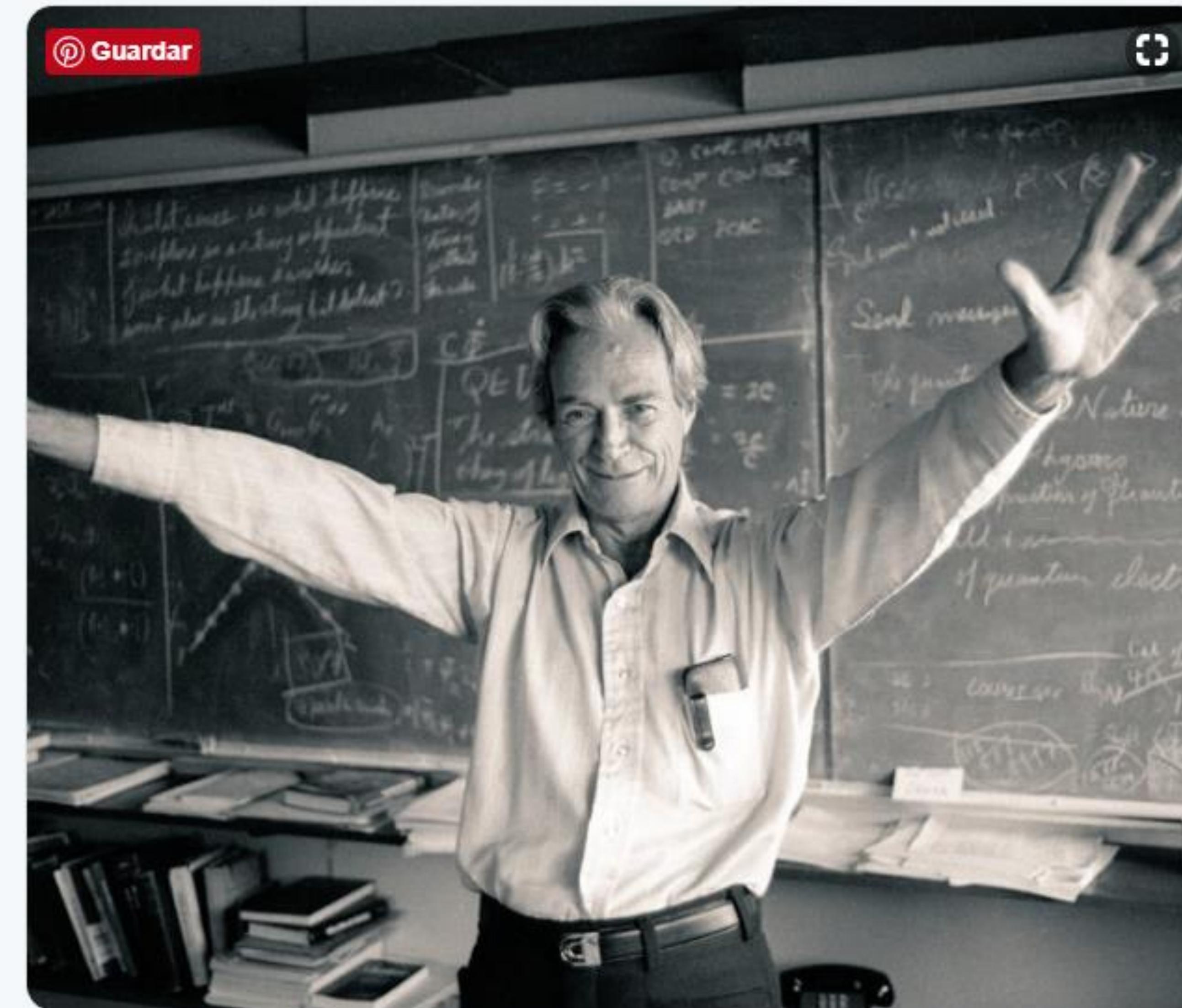




Richard Feynman @ProfFeynman · Oct 10

If you're not having fun, you're not learning. There's a pleasure in finding things out.

80



15



1.5K



3.8K



80

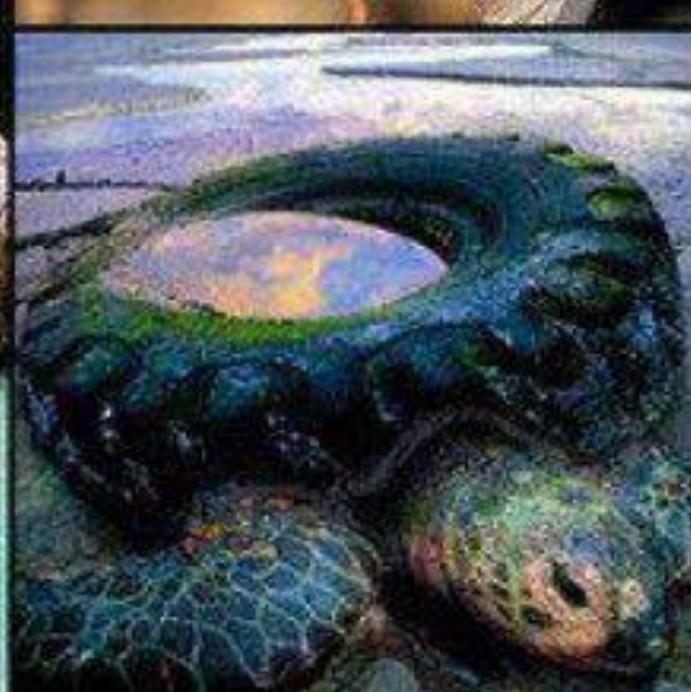
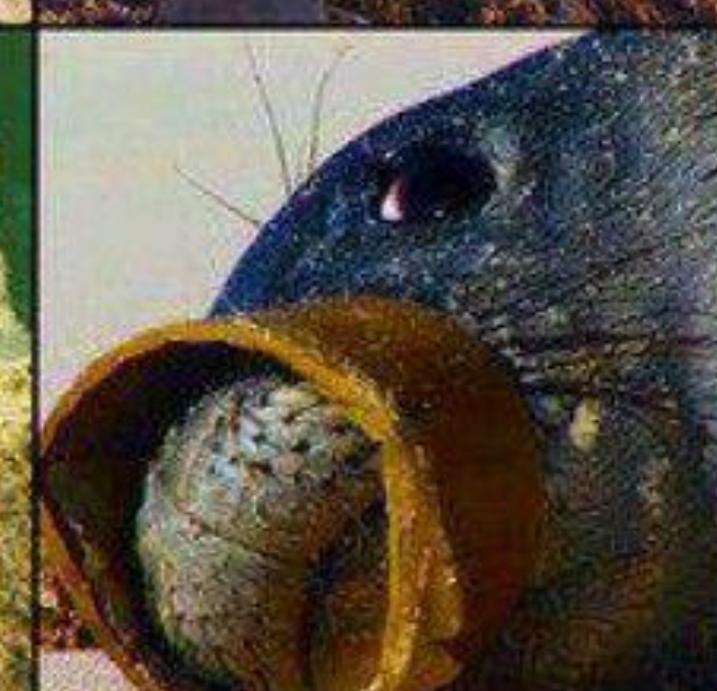
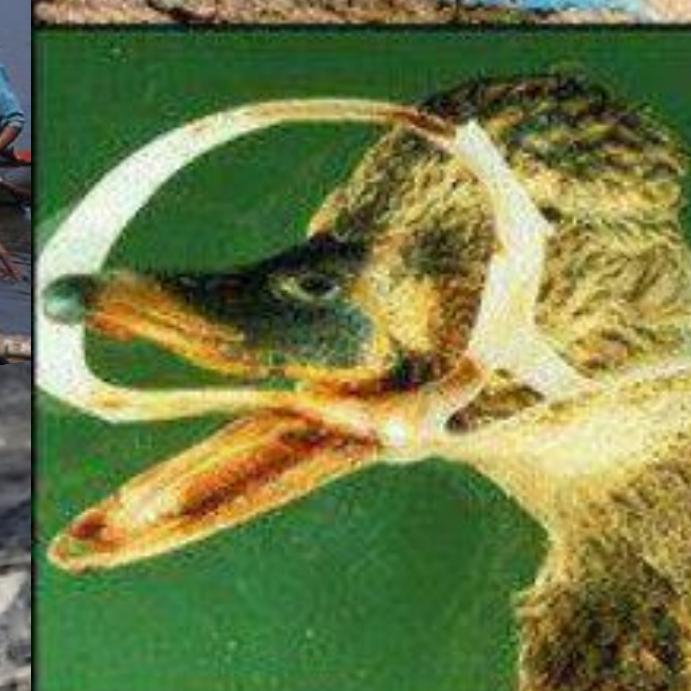
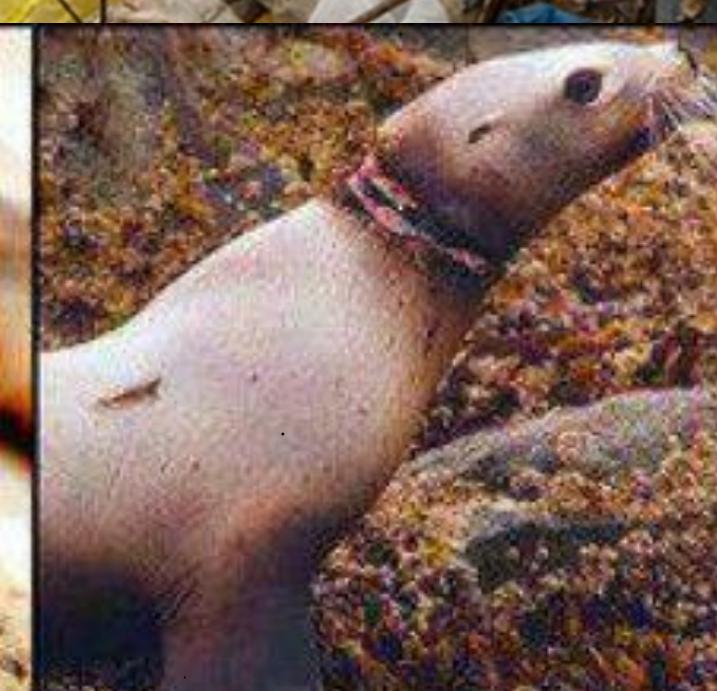
Teamwork:
Together it is
more beautiful.

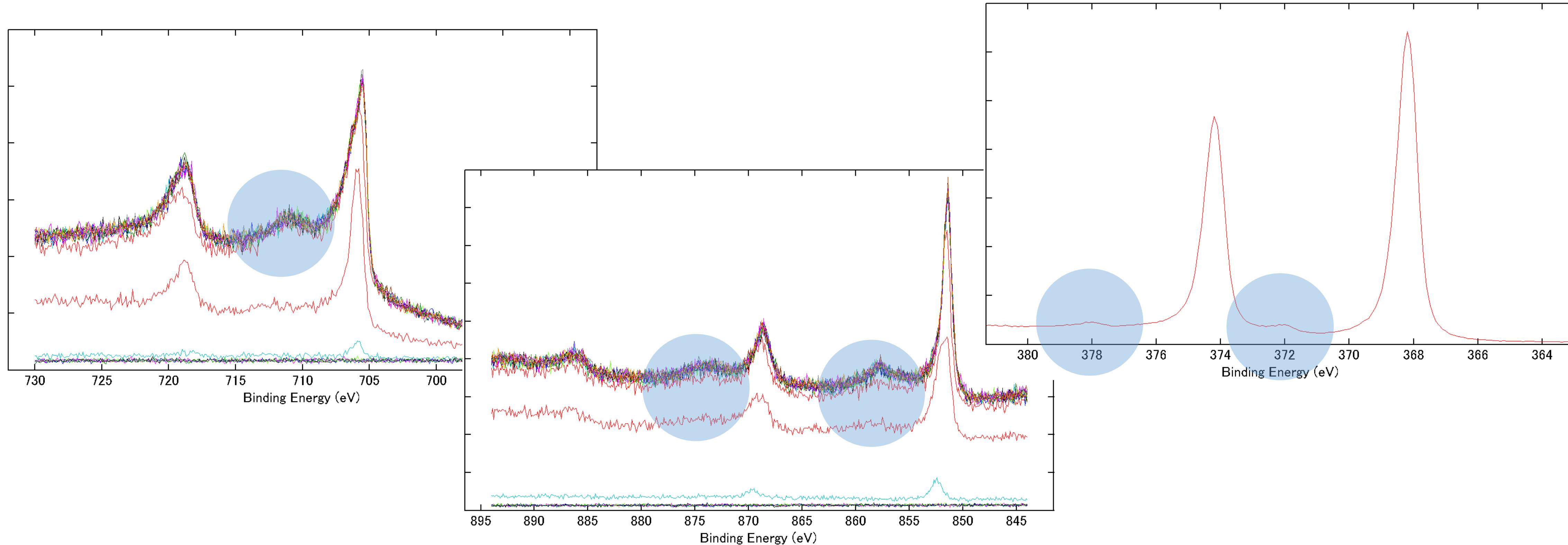


¡Gracias por su atención!

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Los **satélites** también son producto de la **pérdida de energía** por dispersión inelástica producidos en esos tres pasos de la fotoemisión. Estos son efectos de estado final causados por la **relajación** de el sistema después del proceso de fotoemisión.