

Electronic Supplementary Information

Intercalation and grafting of benzene derivatives into Zinc-Aluminum and Copper-Chromium layered double hydroxides hosts: an XPS monitoring.

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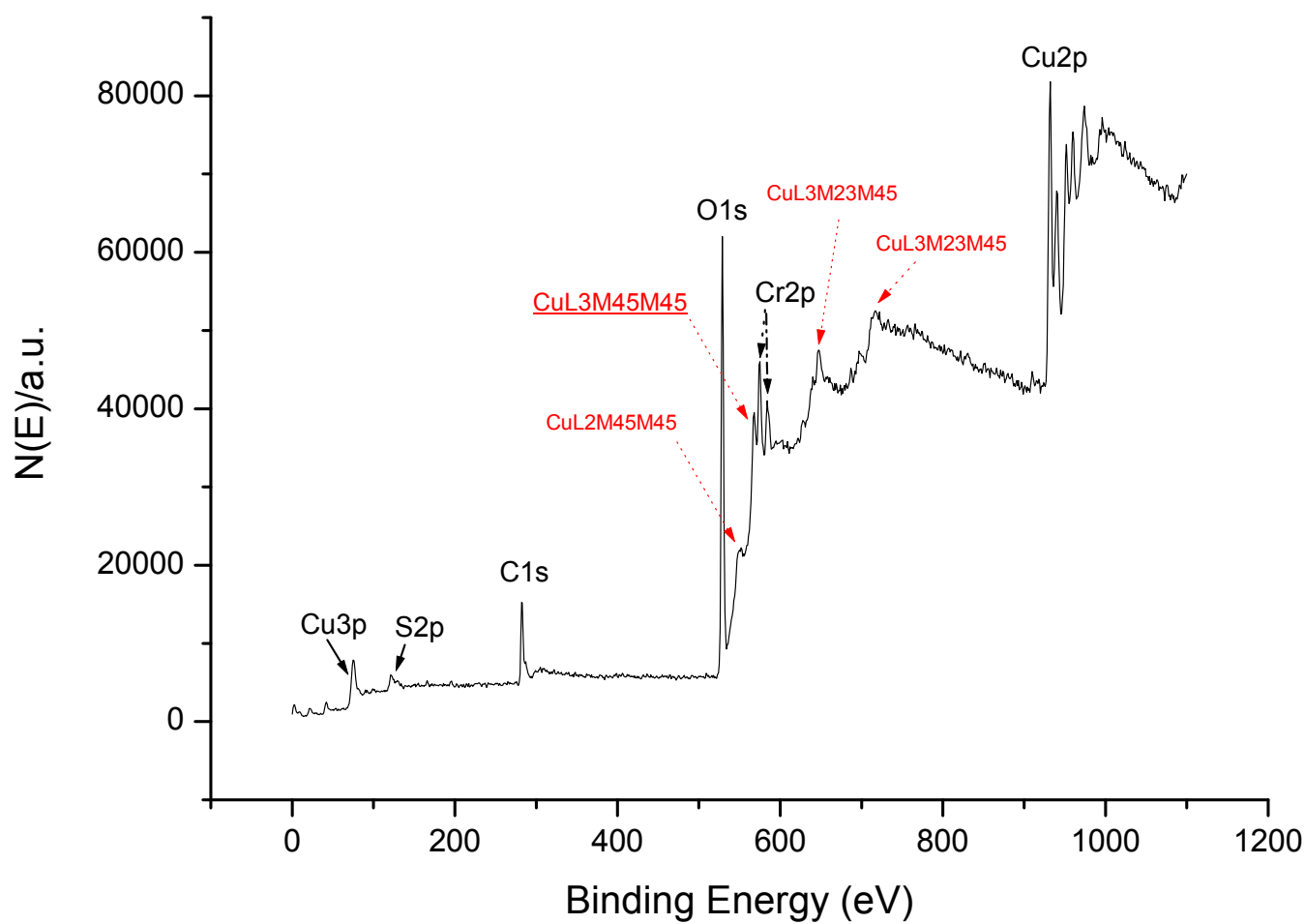


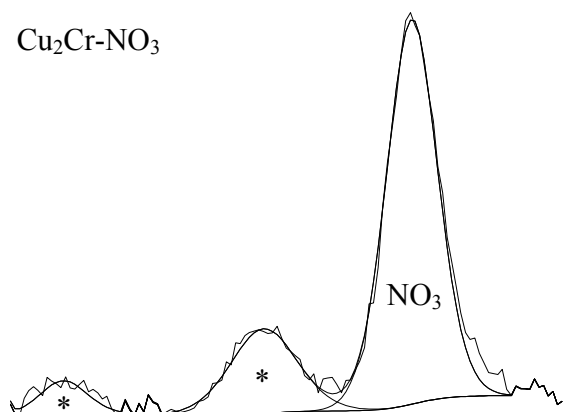
Figure ESI1- Auger lines evidence in Cu₂Cr-HBS XPS survey (RoomT)

a) N1s peak

Cu₂Cr-HBS



Cu₂Cr-NO₃



* : peaks coming from XRay beam reduction of nitrates

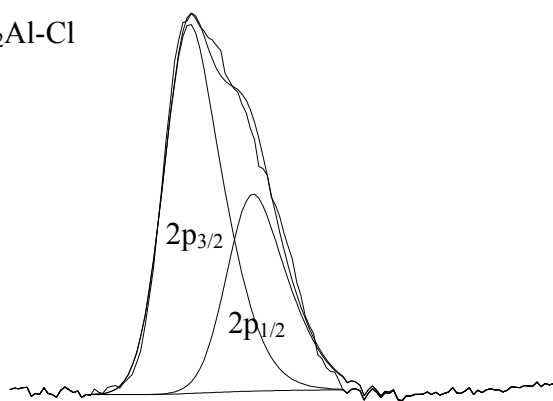
398 400 402 404 406 408 410 412
Binding Energy (eV)

b) Cl2p peak

Zn₂Al-HBS



Zn₂Al-Cl



192 194 196 198 200 202 204 206 208
Binding Energy (eV)

Figure ESI2- a) N1s XPS peak of Cu₂Cr-NO₃ and Cu₂Cr-HBS, and b) Cl2p XPS peak of Zn₂Al-Cl and Zn₂Al-HBS

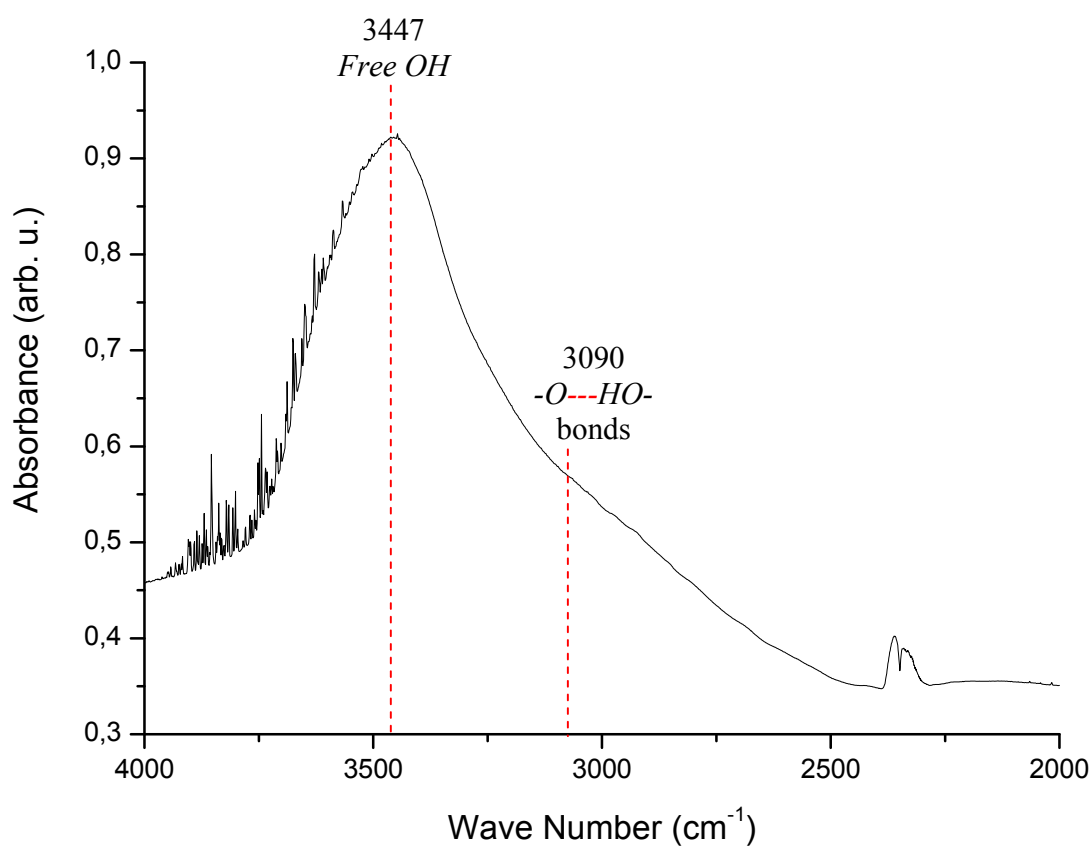


Figure ESI3 – Snapshot of Zn₂Al-HBS FTIR spectrum in the 4000-2000cm⁻¹ region

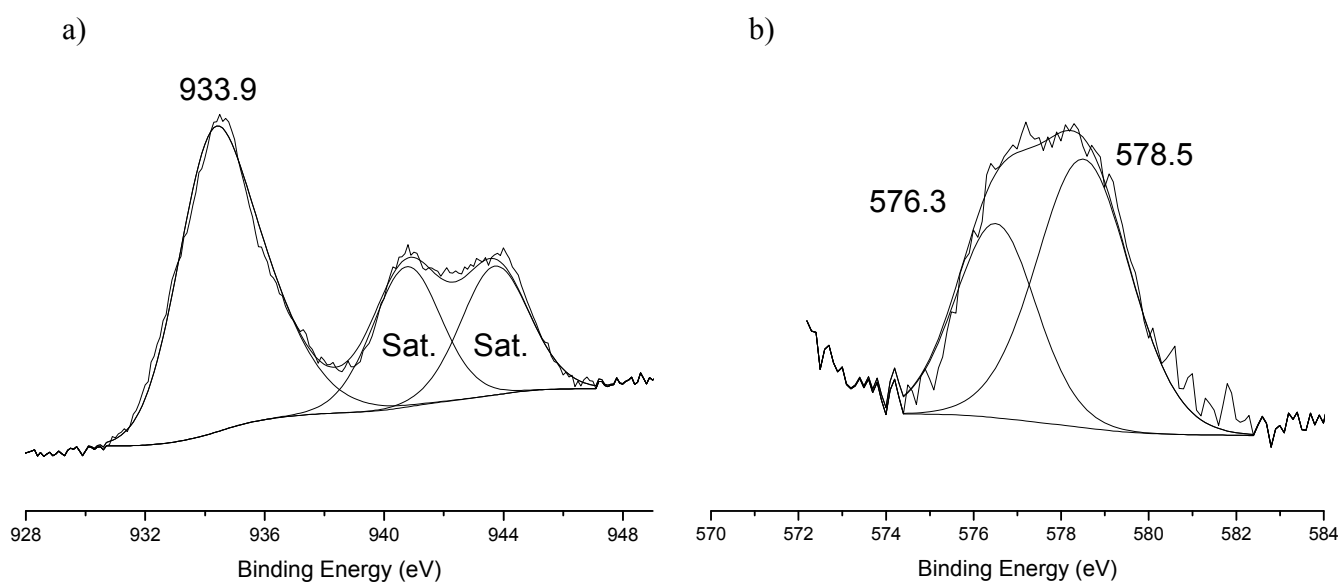


Figure ESI4- XPS peak of Cu₂Cr-HBS at 300°C: a) Cu2p_{3/2} and b) Cr2p_{3/2}

	HBS⁻	HBC⁻	Al(OH)₃	Hybrid system <i>HBS⁻</i> / Al(OH)₃	Hybrid system <i>HBC⁻</i>/ Al(OH)₃	Grafted system <i>HBS⁻</i> - Al(OH)₃	
qS (e⁻)	1.10			1.16		1.25	1.25
qAl (e⁻)			1.07	1.10	1.08	1.16	0.54
qC (e⁻)		0.49			0.52		
qO (e⁻)	-0.86	-0.74	-0.6	-0.58	-0.59	-0.57	-0.53
Over pop S-O (e⁻)	0.313					0.182	0.265
Over pop Al-O (e⁻)			0.260			0.144	0.206
						Single link	Double link

Table ESII- Theoretical calculations of atoms net charges (q) and Mulliken electronic overlapping population (Over pop) for the HBS, HBC organic molecules, a model mineral fragment and the hybrid systems considering the intercalation or the grafting mode.

<i>compound</i> <i>BE region</i>	<i>2CuO,Cr₂O₃</i>	
O1s	529.5 (1.4)	35.0%
	531.1 (1.8)	16.4%
C1s	284.6 (1.3)	28.0%
	287.9 (2.3)	4.7%
Cu 2p_{3/2}	933.9 (3.6)	2.4%
	941.4 (3.1)	1.3%
	944.8 (2.2)	0.7%
Cr2p_{3/2}	576.2 (2.3)	8.4%
	578.5 (2.6)	3.1%

Table ESI2: XPS data of the manufactured (CAS#209317, Aldrich) 2CuO,Cr₂O₃: Binding Energies and FWHM of peaks (in parentheses) are reported in eV and atomic percentage (%).