

Synthesis of single layer graphene on Cu(111) by C₆₀ Supersonic Molecular Beam Epitaxy

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Supporting Information

XPS and UPS analysis

Figure S1 (left panel) shows the Cu2p CL from polycrystalline and (111) copper surfaces. Emission from both surfaces shows the same characteristics, with presence of a 1/2 - 3/2 doublet located at ~952.4 eV and ~932.6 eV (see Table S1), with a 19.8 eV BE distance and the expected intensity ratio (1/2). The estimated Cu2p photoelectron attenuation length is about 1.4 nm, thus the low surface sensitivity does not enable an efficient analysis of the last copper atomic layer (0.2 nm), to have evidence of the proposed seven atom vacancy reconstruction. On the contrary, valence band (VB) curves are very different for the two copper surfaces, reflecting the ordered structure in the Cu(111) case (Figure S1, right panel).

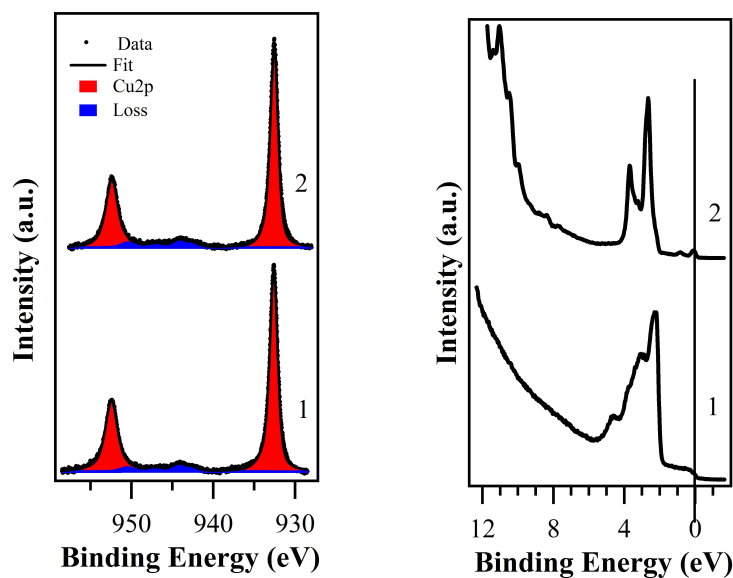


Figure S1 Cu 2p CL (left panel) and VB (right panel) from a clean polycrystalline copper (1) and from a Cu(111) surface (2).

	Cu Polycrystalline			Cu(111)		
	BE [eV]	FWHM [eV]	%	BE [eV]	FWHM [eV]	%
Cu2p 3/2	932.60	1.14	60.7	932.54	1.13	60.9
Cu2p 1/2	952.45	1.73	31.9	952.39	1.69	30.6
Loss	942.70	2.00	1.6	942.64	2.00	1.9
Loss	944.30	2.00	2.7	944.23	2.00	2.9
Loss	947.08	2.00	1.4	947.00	2.00	1.6
Loss	950.51	2.00	1.7	950.43	2.00	2.1

Table S1 Analysis of Cu2p CL from a polycrystalline and a (111) copper surface.

This is evident for the 3d bands, as well as for the Fermi edge region, where presence of surface states dominates VB for the crystalline surface.^{1,2} Figure S2 shows all C1s CL from analyzed C₆₀ film, while in Table S2 and S3 are described components characteristics. As can be seen, C1s core level from all C₆₀ 1 ML films are characterized by the same features (within typical errors), apart from film treated at two higher temperatures. Corresponding VB curves are shown in Figure S3.

Figure S2 a) C1s CL from C₆₀ films deposited by SuMBE on Cu poly at 15 eV KE (1-3) and Cu(111) at 35 eV KE (4, 5) with thickness: 1) 20 nm; 2) 1 ML, after annealing at 430°C of a 20 nm film; 3) 1 ML; 4) 0.3 ML; 5) 0.6 ML. b) C1s from a C₆₀ 1 ML film deposited at RT and precursor 35 eV KE, after thermal annealing at 425°C (6), 645°C (7), 795°C (8). All depositions with substrate at RT. C1s emission from graphene single layer is shown for comparison (9).

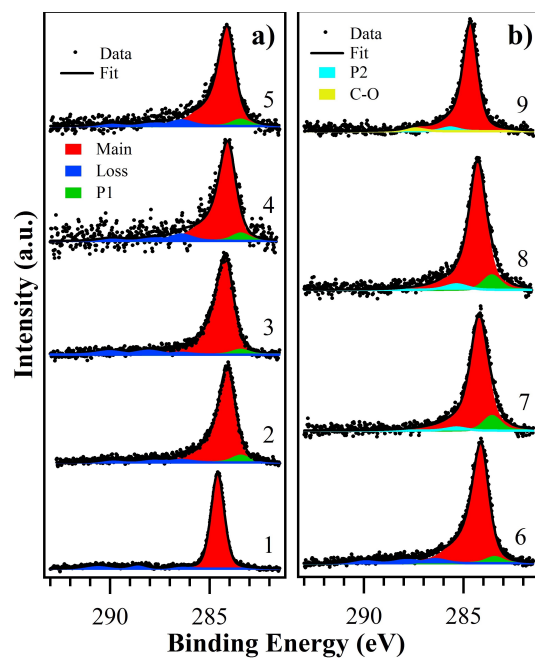


Table S2 Analysis of C1s CL from C₆₀ films with different thickness.

	C ₆₀ Bulk			1ML, Poly Cu, KE=15eV, 400°C			1ML, Cu(111), KE=35eV, RT		
	BE [eV]	FWHM [eV]	%	BE [eV]	FWHM [eV]	%	BE [eV]	FWHM [eV]	%
C-C	284.60	0.80	86.6	284.12	0.90	86.9	284.14	0.92	87.6
P1	286.50	1.00	2.0	283.44	1.00	4.5	283.44	1.00	3.1
Loss	288.60	1.30	4.6	286.41	1.30	2.1	286.41	1.30	2.8
Loss	290.60	1.50	6.8	287.95	1.50	3.5	287.97	1.50	1.6
Loss	284.60	0.80	86.6	289.90	1.50	3.0	289.92	1.50	2.9

	0.3ML, KE=35eV Cu(111)			0.6ML, KE=35eV Cu(111)		
	BE [eV]	FWH M [eV]	%	BE [eV]	FWH M [eV]	%
C-C	284.1 1	0.92	84.1	284. 11	0.92	85.1
P1	283.4 4	1.00	4.5	283. 44	1.00	3.9
Loss	286.4 2	1.30	5.1	286. 41	1.30	4.6
Loss	287.9 4	1.50	3.4	287. 97	1.50	3.4
Loss	289.8 9	1.50	2.9	289. 92	1.50	3.0

Table S3 Analysis of C1s CL from 1 ML C₆₀ film on Cu(111), deposited at RT by SuMBE at 35 eV after different thermal treatments.

	TT @ 425°C				TT @ 645°C			TT @ 795°C			Graphene STD		
	BE [eV]	FWH M [eV]	%		BE [eV]	FWH M [eV]	%	BE [eV]	FWH M [eV]	%	BE [eV]	FWH M [eV]	%
C-C	284.14	0.92	87.6	C-C	284.23	1.03	88.8	284.30	1.00	88.1	284.66	0.88	95.1
P1	283.44	1.00	3.1	P1	283.56	1.00	8.9	283.57	1.00	7.9			
Loss	286.41	1.30	2.8	P2	285.35	1.22	2.3	285.35	1.30	4.0	285.66	1.00	2.7
Loss	287.97	1.50	1.6	C-O							287.40	1.30	2.2
Loss	289.92	1.50	2.9										

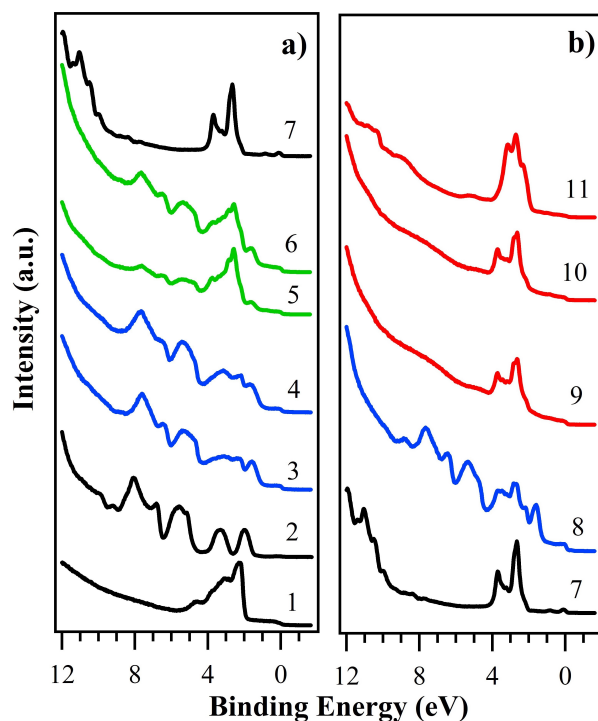


Figure S3 a) Valence band analysis of C_{60} films deposited by SuMBE on Cu poly at 15 eV KE (2-4) and Cu(111) at 35 eV KE (5, 6) with thickness: 1) 20 nm; 3) 1 ML, after annealing at 430°C of a 20 nm film; 4) 1 ML; 5) 0.3 ML; 6) 0.6 ML. b) C1s from a C_{60} 1 ML film deposited at RT and precursor 35 eV KE, after thermal annealing at 425°C (8), 645°C (9), 795°C (10). All depositions were performed keeping the substrate at RT. VB from Cu poly (1), Cu(111) (7) and graphene single layer (10) are shown for comparison.