

Supplementary material

Engineering active sites on reduced graphene oxide by hydrogen plasma irradiation: Mimicking bifunctional metal/supported catalysts in hydrogenation reactions.

Ana Primo,¹ Antonio Franconetti,² Monica Magureanu,³ Nicolae Bogdan Mandache³, Cristina Bucur,⁴ Cristina Rizescu,⁵ Bogdan Cojocaru,⁵ Vasile I. Parvulescu,⁵ Hermenegildo Garcia¹

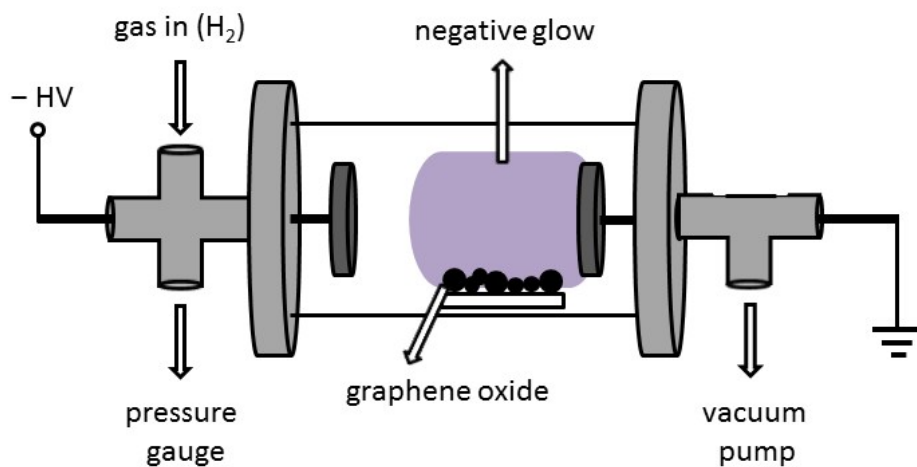
¹Instituto Universitario de Tecnología Química, Universitat Politècnica de València-Consejo Superior de Investigaciones Científicas, Avenida de los Naranjos s/n, 46022 Valencia, Spain

²Departament de Química, Universitat Autònoma de Barcelona, 08193 Cerdanyola del Vallès, Spain

³Department of Plasma Physics and Nuclear Fusion, National Institute for Lasers, Plasma and Radiation Physics, 077125 Magurele, Romania

⁴National Institute of Materials Physics, Atomistilor 105b, 077125 Magurele-Ilfov, Romania

⁵ Department of Organic Chemistry, Biochemistry and Catalysis, Faculty of Chemistry, University of Bucharest, Bdul Regina Elisabeta, 4-12, Bucharest 030016, Romania; vasile.parvulescu@chimie.unibuc.ro



Scheme S1. Scheme of the plasma reactor used for treating graphene.

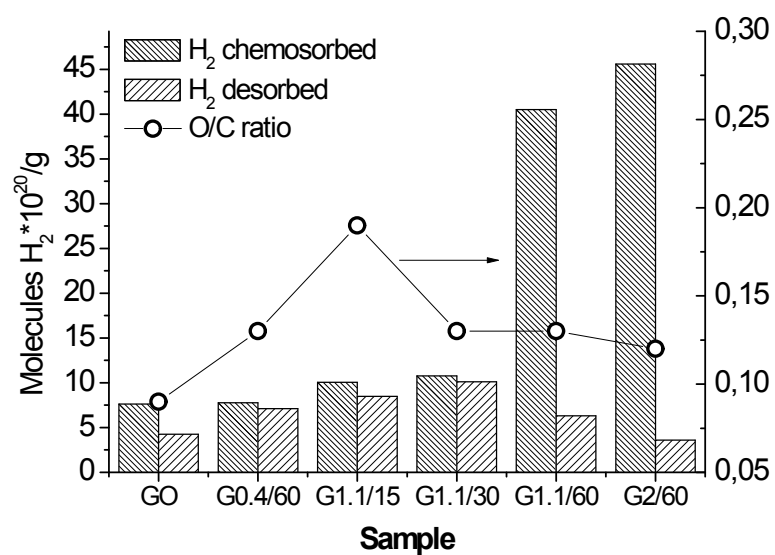


Figure S1. Chemisorbed and desorbed hydrogen vs. the XPS O/C

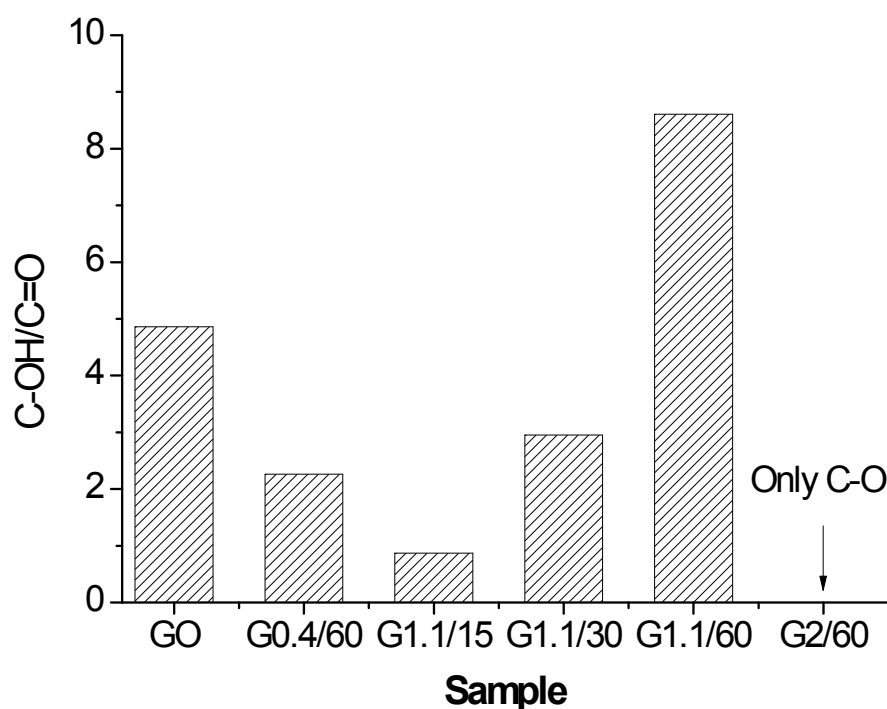


Figure S2. C-O/C=O ratio calculated from the area of the deconvoluted bands from the C 1s levels.

Table S1. Summary of the binding energy and intensity of the main components obtained from the deconvolution fitting of the XPS C1s and O1s peaks for each of the graphene samples under study.

	RGO		G0.4/60		G1.1/15		G1.1/30		G1.1/60		G2/60	
BE _x (eV) A _x (cps*eV)	O1s	C1s	O1s	C1s	O1s	C1s	O1s	C1s	O1s	C1s	O1s	C1s
BE1	533.6	285.2	532.1	285.2	532.2	284.1	532.4	288.2	532.1	285.3	532.1	285.1
A1	920.0	5403.4	1320.8	5900.7	4987.1	7304.7	2725.1	444.1	1052.3	5382.7	1301.1	6591.0
BE2	532.4	284.5	533.6	284.6	533.4	285.5	533.7	284.6	533.7	284.6	533.6	284.5
A2	2501.1	2772.1	3594.2	3402.5	2206.0	1279.9	633.9	19434.3	3203.7	33062.1	3512.9	33361.5
BE3	534.8	285.8		286.9		284.5		286.5		287.0		286.6
A3	150.5	15192.1		1296.9		16805.1		1310.8		941.4		1328.9
BE4		286.6	530.9	286.1	530.6	288.7	530.9	285.4	530.9	286.1	530.9	286.0
A4		845.3	921.4	4304.2	367.8	2360.0	646.0	5611.6	762.9	3877.5	884.2	3427.8
BE5		289.2	535.9	288.3		285.0		292.7	535.7	288.4		
A5		3297.1	151.1	604.3		9269.6		3902.4	902.7	450.3		
BE6						286.3						
A6						2066.2						
TOTAL Amplitude	3571.6	38786.0	5987.5	46131.1	7561.0	39085.6	4005.1	30703.1	5921.5	43714.1	5698.2	44709.2

Ratio O/C	0.09	0.13	0.19	0.13	0.14	0.13
--------------	------	------	------	------	------	------

Ai- area of the deconvoluted peaks; BE- binding energy

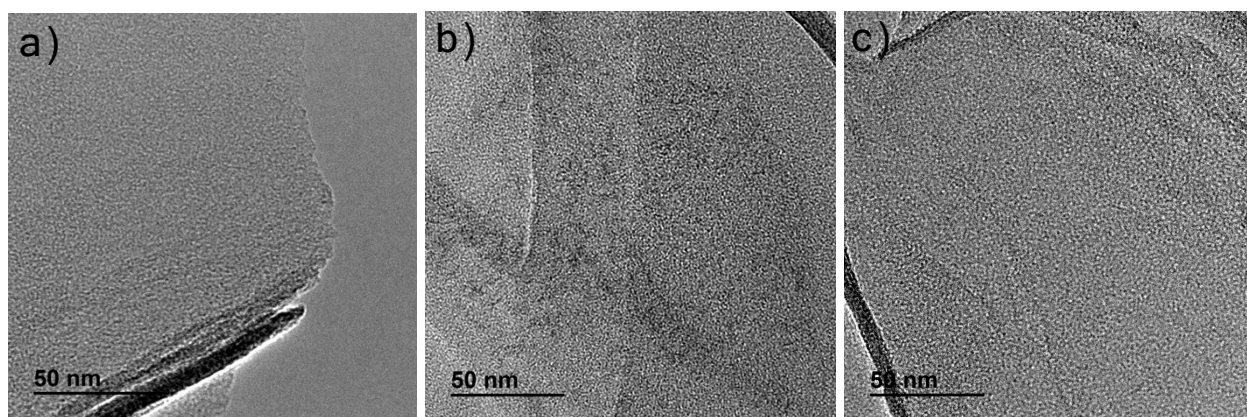


Figure S3. TEM images of G1,1/15, G1,1/60 and G2/60 at the same magnification. The white spots are corresponding to the defects on the sheet.

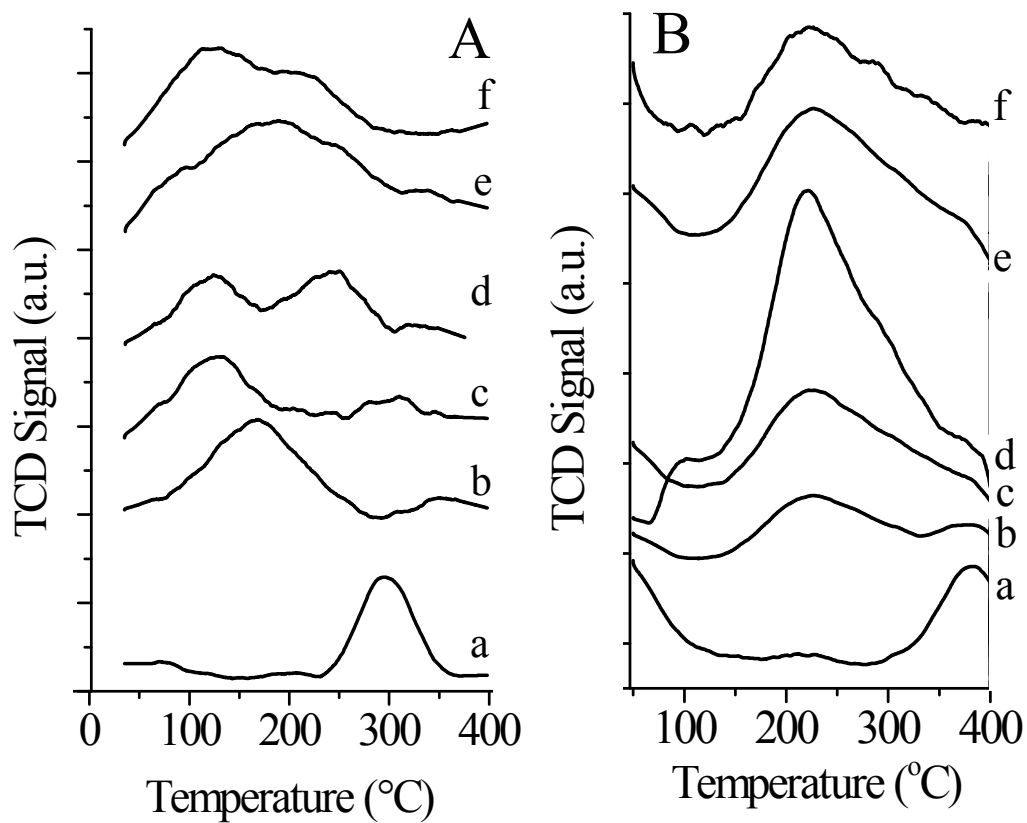


Figure S4. TPD-H₂ (A) and TPD-NH₃ (B) for a) RGO, b) G0.4/60, c) G1.1/15, d) G1.1/30, e) G1.1/60, f) G2/60.