

Supplemental information

Alterations in the surface features of S-doped carbon and g-C₃N₄ photocatalysts in the presence of CO₂ and water upon visible light exposure

Wanlu Li ^{a,b}, Yuping Hu^{a, c}, Enrique Rodríguez-Castellón^{d*} and T. J. Bandosz ^{a,b*}

a. Department of Chemistry and Biochemistry, The City College of New York, New York, NY 10031, USA.

b. Ph.D. Program in Chemistry, The Graduate Center of the City University of New York, New York, NY 10016 USA.

c. On leave from College of Chemistry and Chemical Engineering Guangxi University for Nationalities, Nanning, 530006 China and Guangxi Key Laboratory of Chemistry and Engineering of Forest Products, Nanning, 530006, China.

d. Departamento de Química Inorgánica, Facultad de Ciencias, Universidad de Málaga, Málaga, 29071, Spain.

* Whom correspondence should be addressed to: Tel; (212) 650-607; Fax: (212) 650-6107;
tbandosz@ccny.cuny.edu

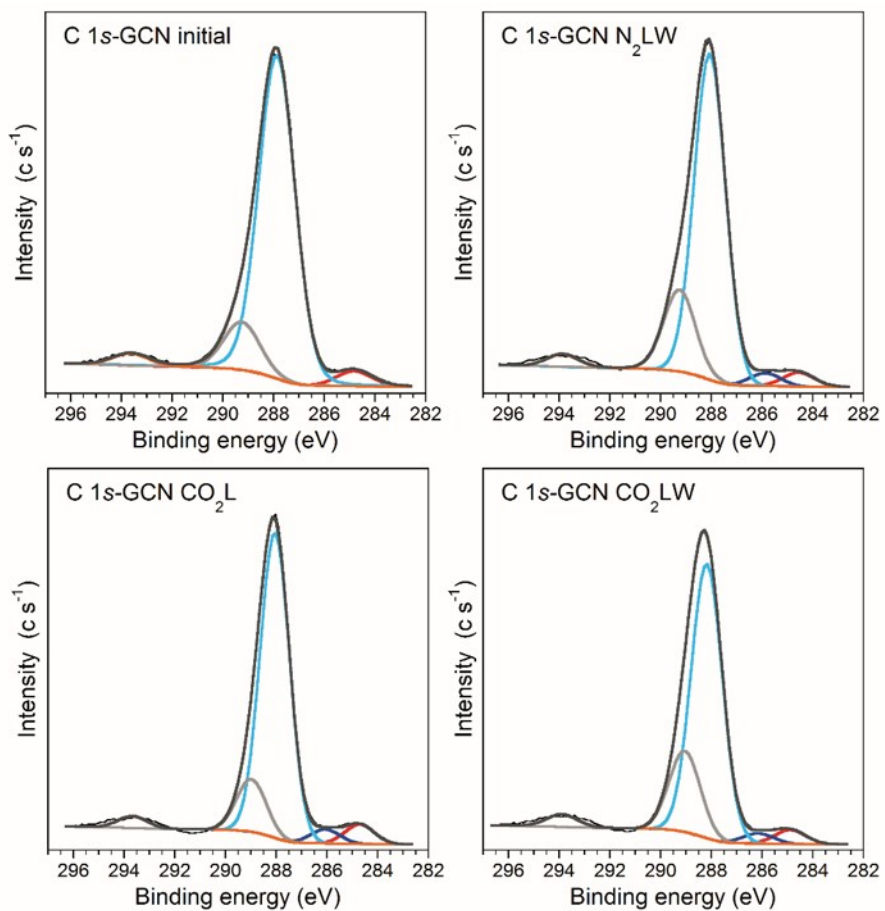


Figure S1. Deconvolution of C1s core energy levels for the GCN samples.

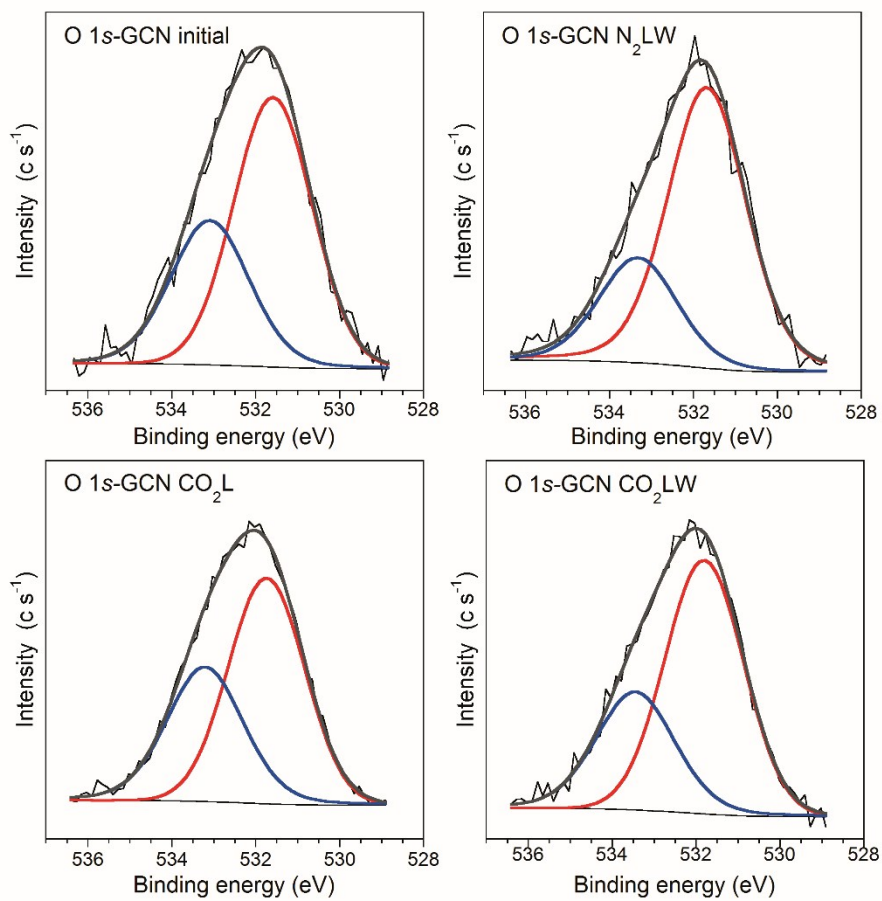


Figure S2. Deconvolution of O1s core energy levels for the GCN samples.

Table S1. Surface pH values, peak positions and numbers of groups (in parentheses, [mmol/g]) for GCN in different conditions.

Sample	Surface pH	pK _a 4-5	pK _a 5-6	pK _a 6-7	pK _a 7-8	pK _a 8-9	pK _a 9-10	All
GCN-initial	7.07			6.23 (0.042)			9.07 (0.057)	0.099
GCN-CO ₂ LW	6.59			6.17 (0.029)			9.02 (0.033)	0.062
GCN-CO ₂ DW	6.53	4.35 (0.001)		6.54 (0.047)				0.048
GCN-N ₂ LW	6.86		5.52 (0.031)			8.80 (0.051)		0.082
GCN-N ₂ DW	6.92				7.08 (0.048)			0.048
GCN-CO ₂ L	6.85	4.20 (0.006)			7.68 (0.031)			0.037
GCN-CO ₂ D	6.43			6.08 (0.029)		8.32 (0.019)		0.048
GCN-N ₂ L	6.29	4.33 (0.019)				8.06 (0.036)		0.055

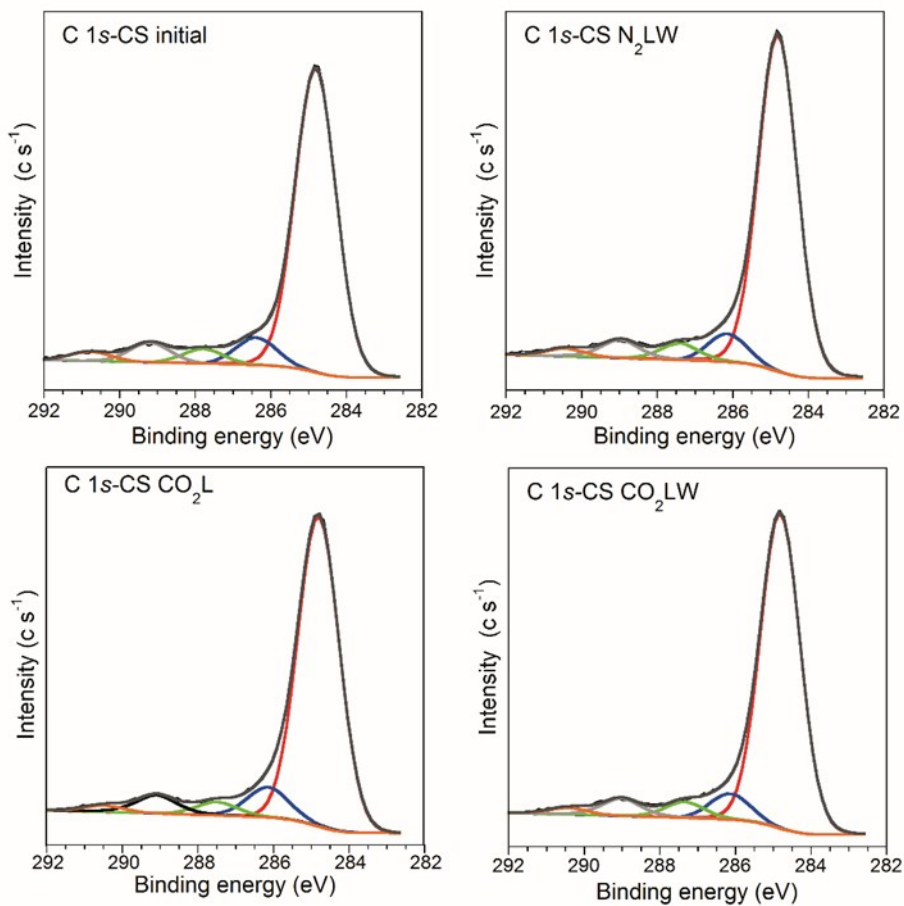


Figure S3. Deconvolution of C1s core energy levels for the CS samples

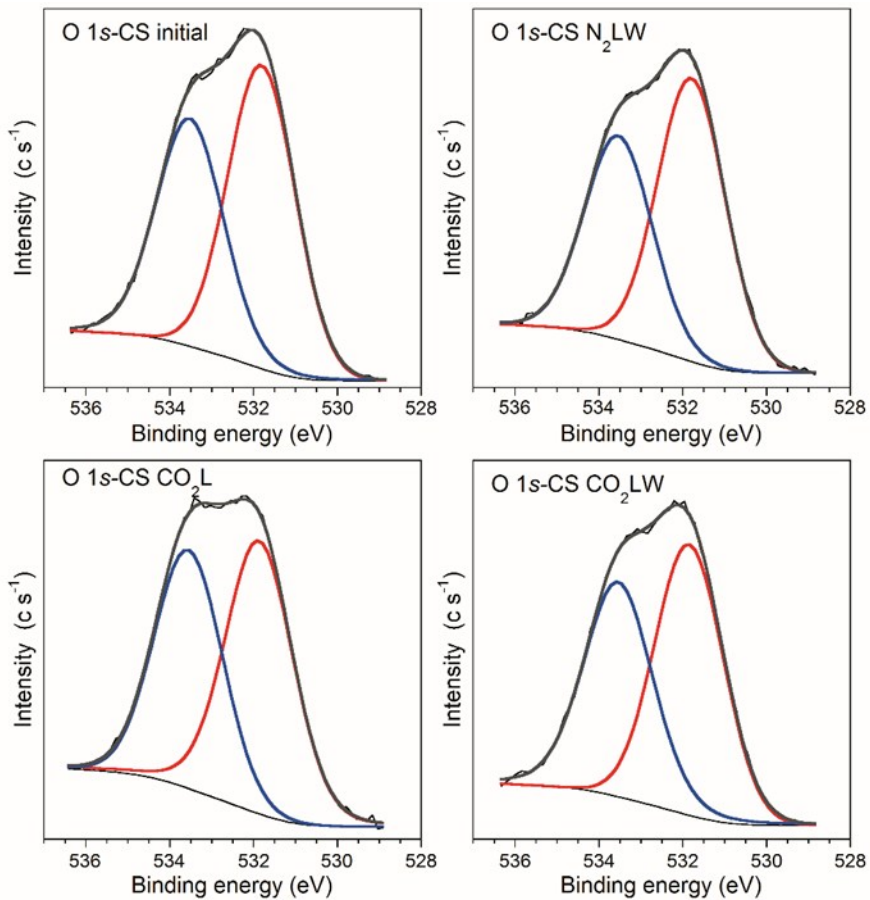


Figure S4. Deconvolution of O1s core energy levels for the CS samples.

Table S2. Surface pH values, peak positions and numbers of groups (in parentheses, [mmol/g]) for CS in different conditions.

Sample	Surface pH	pK _a 4-5	pK _a 5-6	pK _a 6-7	pK _a 7-8	pK _a 8-9	pK _a 9-10	All
CS-initial	3.16	4.22 (0.084)	5.59 (0.068)		7.77 (0.081)		9.57 (0.115)	0.347
CS-CO ₂ LW	3.20	4.94 (0.067)		6.65 (0.069)	7.91 (0.038)		9.5 (0.127)	0.301
CS-CO ₂ DW	3.25		5.42 (0.084)		7.69 (0.055)		9.44 (0.082)	0.221
CS-N ₂ LW	3.15		5.10 (0.089)		7.39 (0.074)		9.41 (0.087)	0.250
CS-N ₂ DW	3.20		5.20 (0.078)		7.702 (0.074)		9.66 (0.097)	0.249
CS-CO ₂ L	3.01	4.87 (0.084)		6.38 (0.085)		8.33 (0.075)	9.38 (0.067)	0.310
CS-CO ₂ D	3.08	4.53 (0.065)	5.77 (0.064)		7.72 (0.072)		9.51 (0.111)	0.311
CS-N ₂ L	3.02	4.40 (0.086)		6.00 (0.100)		8.05 (0.092)	9.85 (0.085)	0.363

Table S3. The parameters of the porous structure for CS in different conditions.

Sample	S _{BET} (m ² /g)	V _t (cm ³ /g)	V _{meso} (cm ³ /g)	V _{<0.7nm} (cm ³ /g)	V _{<1nm} (cm ³ /g)	V _{mic} (cm ³ /g)	V _{mic} / V _t
CS-intial	395	0.392	0.239	0.130	0.141	0.153	0.39
CS-CO ₂ LW	345	0.368	0.229	0.113	0.124	0.139	0.38
CS-CO ₂ DW	382	0.414	0.266	0.122	0.129	0.148	0.36
CS-N ₂ LW	416	0.432	0.279	0.123	0.133	0.153	0.35
CS-N ₂ DW	380	0.400	0.245	0.133	0.140	0.155	0.39
CS-CO ₂ L	400	0.391	0.236	0.133	0.139	0.155	0.40
CS-N ₂ L	384	0.371	0.220	0.129	0.134	0.151	0.41
CS-CO ₂ D	379	0.362	0.214	0.111	0.140	0.148	0.41