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Supporting information for article:

Intercalated water in multi-layered graphene oxide paper: an X-ray scattering study

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Supporting information

Supporting information (such as experimental data, additional figures and multimedia content) that may be of use or interest to some readers but does not form part of the article itself will be made available from the IUCr archives and appropriate databases. If possible, please include supporting material here; otherwise, separate supporting files may be uploaded upon submission of your article.

Table S1 Values obtained by fitting with a Gaussian lineshape function the simulated 001 reflection of GO according to Eq.(4), with parameters $p = 0.8$, $B = 0.5 \text{ \AA}$ ($B = 0$ for values in parentheses).

N	$Q_{001} (\text{\AA}^{-1})$	FWHM (\AA^{-1})
2	0.908 (0.923)	0.42 (0.43)
3	0.976 (0.984)	0.29 (0.29)
4	1.000 (1.004)	0.22 (0.22)
5	1.011 (1.014)	0.17 (0.17)
10	1.025 (1.026)	0.09 (0.09)

Table S2 Values obtained by fitting with a Gaussian lineshape function the simulated 001_{gr} graphitic reflection, with stacking disorder parameter $B = 0.5 \text{ \AA}$ ($B=0$ for values in parentheses).

N	d(\AA)	$Q_{001} (\text{\AA}^{-1})$	FWHM (\AA^{-1})
3	3.40	1.768 (1.816)	0.54 (0.55)
3	3.45	1.744 (1.79)	0.53 (0.54)
3	3.50	1.720 (1.765)	0.53 (0.53)
4	3.40	1.805 (1.831)	0.39 (0.40)
4	3.45	1.780 (1.805)	0.39 (0.39)
4	3.50	1.756 (1.779)	0.38 (0.39)
5	3.40	1.821 (1.837)	0.31 (0.32)
5	3.45	1.795 (1.811)	0.31 (0.31)
5	3.50	1.770 (1.785)	0.31 (0.31)

Physical-chemical characterization

Thermogravimetric analyses (TGA)

Thermogravimetric analyses (TGA) for papers of GO and RGO (GO heat treated at 220 °C for 30 min.) are shown in Fig. S1. TGA studies were performed in a SETARAM Setsys Evolution apparatus. The paper samples were heated with a constant ramp of 10 °C/min until 800 °C under an argon flow of 50 mL/min. Two important weight losses are observed in the region from 30 °C to 130 °C and between 130 °C to 260 °C. The first is assigned to the desorption of physisorbed water intercalated in between the GO sheets, while the second weight loss is attributed to the decomposition of oxygen functional groups (OFGs) and the loss of bound water (Stankovich et al., 2007; Núñez 2015; Núñez et al. 2017). For GO, weight losses of 15 wt. % and 22.5 wt. % are observed for the two temperature ranges, respectively. For rGO, the weight losses are substantially lower, and correspond to 4.5 wt. % and 3 wt. %, respectively.

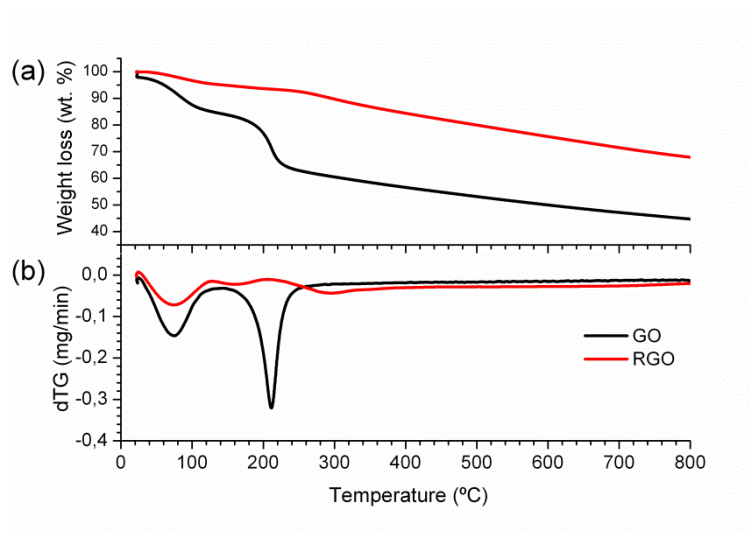


Figure S1 TGA curves for GO and RGO papers. (a) the relative thermogravimetric weight loss and (b) derivative curve of the thermogravimetric weight loss (dTG).

X-ray photoelectron spectroscopy (XPS)

XPS spectra in Fig. S2 show the deconvoluted C1s and core shell spectra for GO and RGO papers. GO is characterized by a relatively low sp^2 C=C contribution and a dominating broad distribution of C-O, C-O-C oxygen functional groups (OFGs), indicative of GO's highly defective structure. When heated to 220 °C, resulting RGO shows a significant decrease of these types of OFGs, which goes along with the decrease of bound water as observed by TGA.

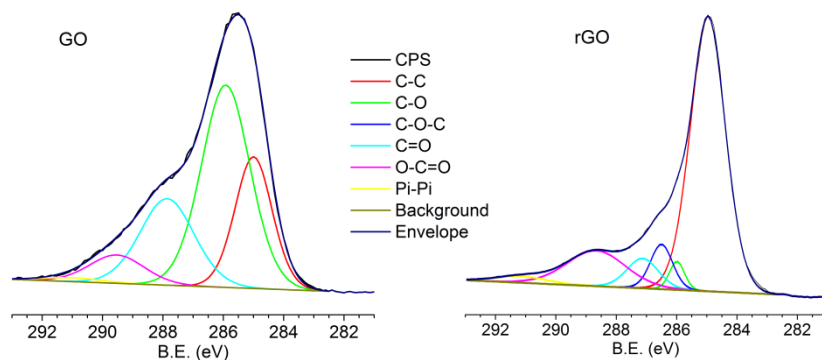


Figure S2 XPS C1s core shell spectra for GO and RGO and the deconvoluted contributions of the various oxygen functional groups.

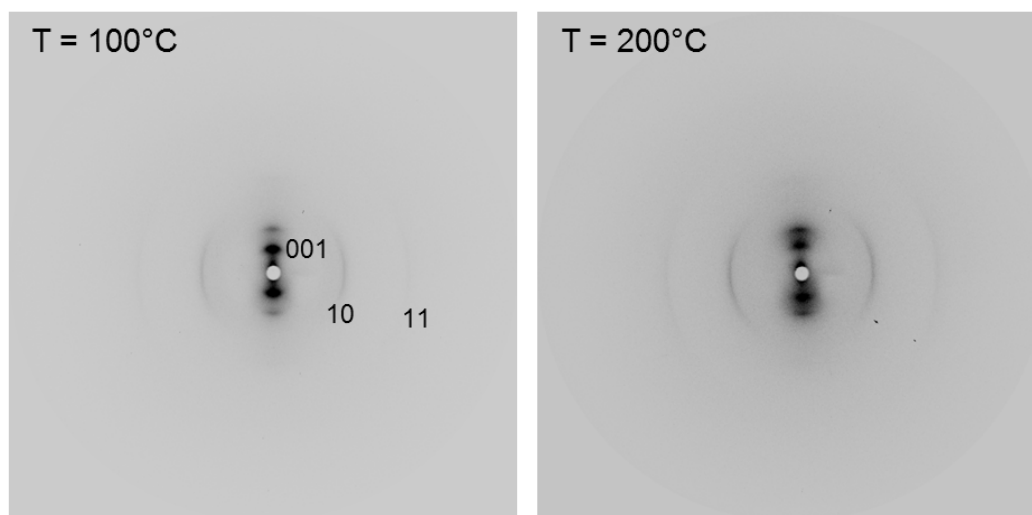


Figure S3 XRS images of GO paper under vacuum taken at T=100°C and T=200°C.

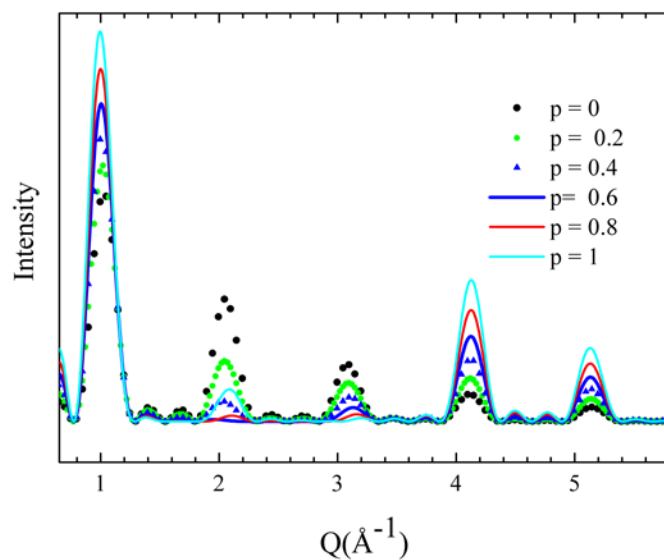


Figure S4 Simulated XRS 00L diagrams of GO for different values of the ratio O:C, named p , with average number of layers fixed $N = 4$, and $B = 0$ (no disorder).

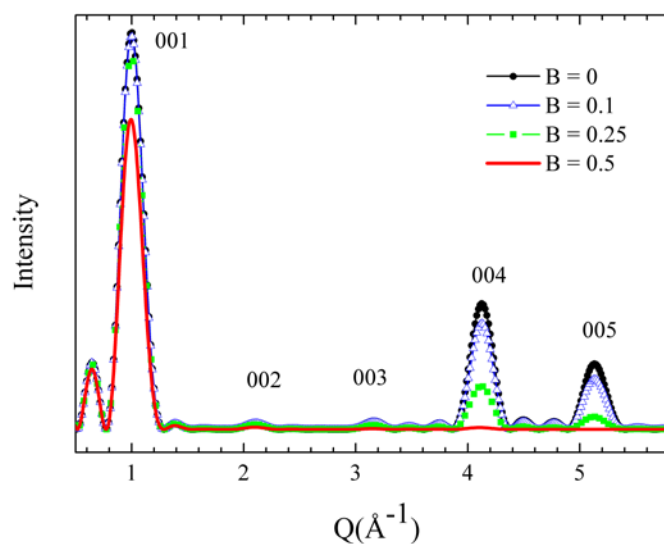


Figure S5 Simulated XRS 00L diagrams of GO by varying the stacking disorder parameter B , with fixed parameters $N = 4$, $p = 0.8$.

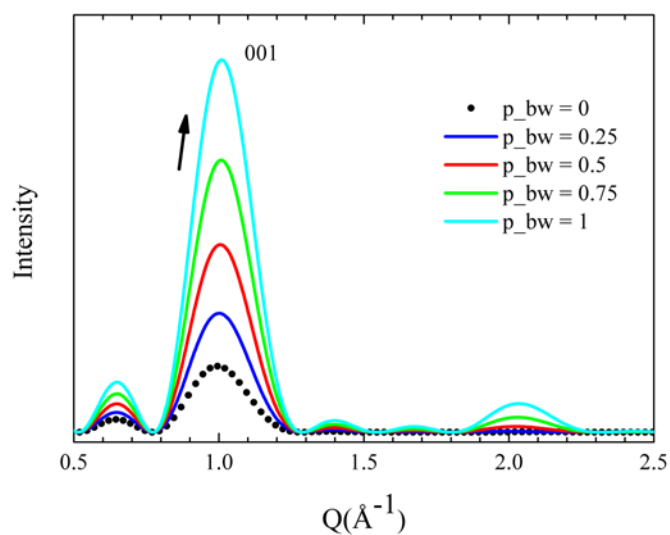


Figure S6 Simulated XRS 00L diagrams of GO with bound water layer at $z_{bw}=0$ (corresponding to bound water in holes, $p_h = 1$) as a function of the ratio p_{bw} of bound water to carbon according to Eq. (6), with fixed parameters $N = 4$, $p = 0.8$, $B = 0.5 \text{ \AA}$.