

## The degree of oxidation of graphene oxide: Supplementary Information

A. Carvalho

*Centre for Advanced 2D Materials, National University of Singapore, 117542 Singapore\**

M. C. F. Costa

*Centre for Advanced 2D Materials, National University of Singapore, 117542 Singapore and  
Materials Science and Engineering, National University of Singapore, 117575 Singapore*

V. S. Marangoni

*Centre for Advanced 2D Materials, National University of Singapore, 117542 Singapore*

Ng Pei Rou

*Centre for Advanced 2D Materials, National University of Singapore, 117542 Singapore*

Nguyen Thi Le Hang

*Centre for Advanced 2D Materials, National University of Singapore, 117542 Singapore*

A. H. Castro Neto

*Centre for Advanced 2D Materials, National University of Singapore, 117542 Singapore and  
Materials Science and Engineering, National University of Singapore, 117575 Singapore*

---

\*Electronic address: [carvalho@nus.edu.sg](mailto:carvalho@nus.edu.sg)

## S1. XPS

TABLE S1: Binding energy (eV) of the deconvoluted C1s XPS peaks and their relative percentage area (in parentheses) for graphene and GO with different oxidation degree. Oxygen percentages were obtained from the Survey spectra.

Sample	[O](%)	C=C ( $sp^2$ )	C-C ( $sp^3$ )	C-O	C=O	O-C=O	$\pi-\pi^*$
Graphene	18.1	284.76 (81.8%)	285.30 (10.5%)	286.24 (2.8%)	286.99 (1.4%)	287.77 (0.7%)	290.90 (2.8%)
GO #1	25.7	284.60 (26.7%)	285.15 (33.6%)	287.01 (33.5%)	288.17 (4.0%)	289.10 (2.1%)	
GO #2	32.2	284.82 (22.1%)	285.77 (29.4%)	287.71 (40.4%)	288.93 (4.9%)	289.86 (3.2%)	
GO #3	33.5	284.94 (9.4%)	286.26 (34.3%)	288.39 (46.6%)	288.79 (5.3%)	290.26 (4.4%)	

## S2. XPS of edge carbonyl in GO

The C1s core level shifts for the carbon nearest to an edge carbonyl were calculated using the edge model (Fig. 2). The oxygen content of the graphene oxide was modelled by parallel oriented epoxy oxygen, occupying randomly the sites represented as crossed red circles in the figure. Edge terminating atoms were not considered in the calculation of the oxygen concentration.

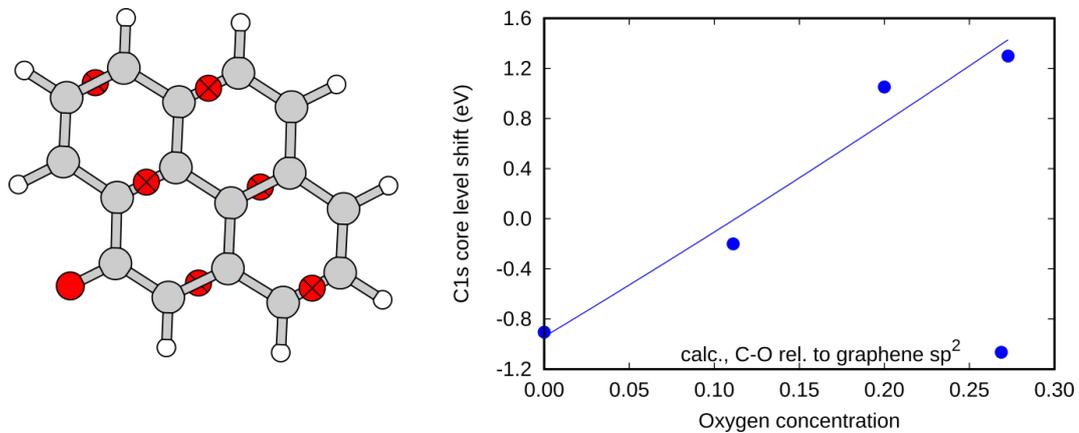


FIG. 1: C1s core level shifts vs. concentration for the edge carbonyl ( $=O$ ), represented as a red circle on the left. Crossed red circles represent oxygen atoms added to increase the oxygen concentration.

## S3. Fourier Transform Infra-Red (FTIR) spectra

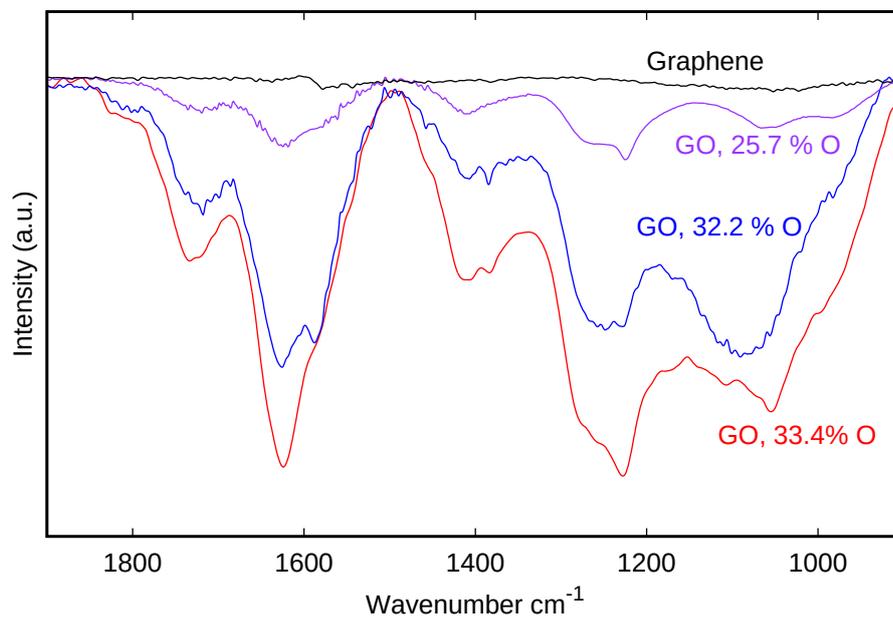


FIG. 2: FTIR spectra for the graphene and graphene oxide samples with different oxygen concentrations.

The FTIR spectra are typical for graphene oxide structures and are normalized with respect to the highest intensity band at  $3400\text{ cm}^{-1}$  (which are hydrogen-related, and are not shown). The resonances at  $1054$ ,  $1260$  and  $1418\text{ cm}^{-1}$  are attributed to the C-OH stretching, C-O stretching and O-H deformation vibrations, respectively. The  $1260\text{ cm}^{-1}$  is the epoxy symmetric stretch.