

## Electronic Supplementary Information (ESI)

# Characterization of Hydrogenated Graphite Powder by X-ray Photoelectron Spectroscopy and Time-of-Flight Secondary Ion Mass Spectrometry

Wenjing Xie,<sup>a</sup> Kai Mo Ng,<sup>b</sup> Lu-Tao Weng<sup>cd</sup> and Chi-Ming Chan<sup>\*ac</sup>

<sup>a</sup> Division of Environment

<sup>b</sup> Advanced Engineering Materials Facility

<sup>c</sup> Department of Chemical and Biomolecular Engineering

<sup>d</sup> Materials Characterization and Preparation Facility

Hong Kong University of Science and Technology

Clear Water Bay, Kowloon

Hong Kong

\* Corresponding author.

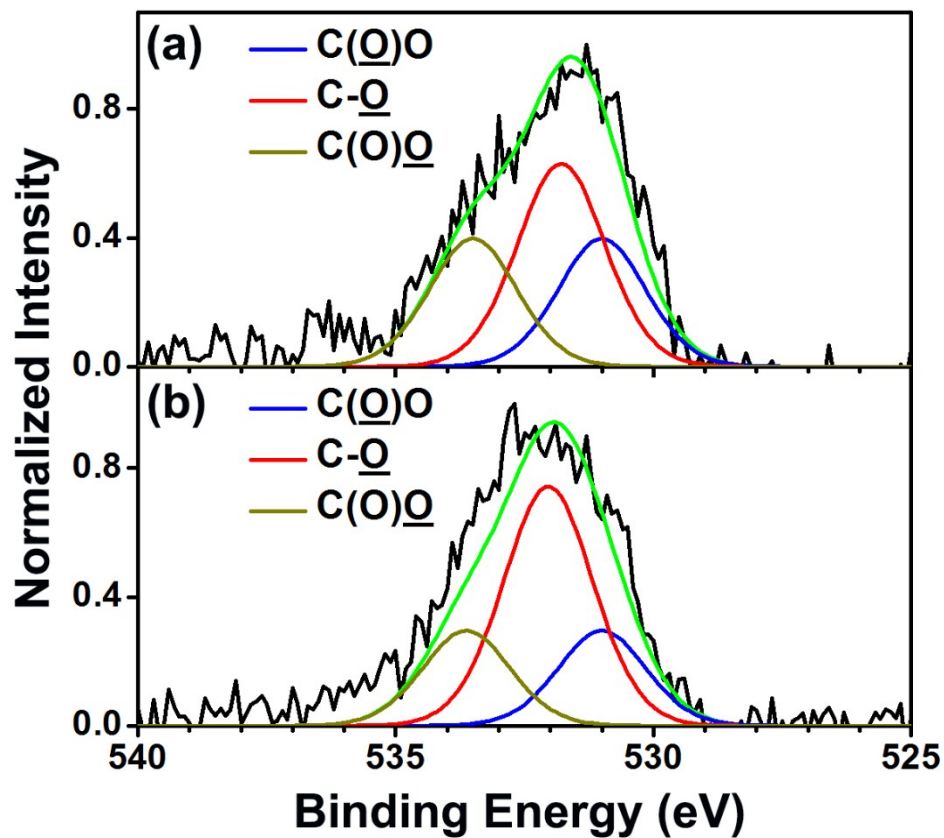
E-mail address: [kecmchan@ust.hk](mailto:kecmchan@ust.hk) (C.M. Chan)

**Table S1** Results of a peak synthesis of the C1s peak of graphite powder and hydrogenated graphite powder

Sample	Peak	Binding Energy (eV)	Area Ratio (%)	FWHM (eV)
Graphite powder annealed at 500 °C	Total C1s	284.6	100.0	1.0
	C-C (sp <sup>2</sup> )	284.6	80.1	0.8
	C-C (sp <sup>3</sup> )	285.2	7.2	1.0
	C-O	286.5	2.5	1.0
	C(O)O	288.0	1.1	1.0
	$\pi$ - $\pi^*$ shake-up	291.0	9.1	3.1
Hydrogenated graphite powder annealed at 500 °C	Total C1s	285.0	100.0	1.3
	C-C (sp <sup>2</sup> )	284.6	39.2	0.8
	C-C (sp <sup>3</sup> )	285.2	51.8	1.0
	C-O	286.5	3.6	1.0
	C(O)O	288.0	1.0	1.0
	$\pi$ - $\pi^*$ shake-up	290.8	4.4	3.1

**Table S2** Residual standard derivation of C1s curve-fitting of graphite powder and hydrogenated graphite powder

Sample	No.	Binding energy of sp <sup>3</sup> carbons (eV)	Residual Standard Deviation
Graphite powder annealed at 500 °C	1	285.1	4.350
	2	285.2	4.347
	3	285.3	4.387
	4	285.4	4.366
	5	285.5	4.376
Hydrogenated graphite powder annealed at 500 °C	1	285.1	3.801
	2	285.2	2.595
	3	285.3	2.726
	4	285.4	4.186
	5	285.5	6.442



**Fig. S1** (a) XPS O1s normalized spectra of graphite powder after 500 °C annealing and (b) hydrogenated graphite powder after 500 °C annealing. The black (—) and green (—) lines represent the experimental and curve-fitted spectra, respectively. Both spectra were obtained at 500 °C.

**Table S3** Results of a peak synthesis of the O1s peak of graphite powder and hydrogenated graphite powder

Sample	Peak	Binding Energy (eV)	Area Ratio (%)	FWHM (eV)
Graphite powder annealed at 500 °C	Total O1s	531.6	100.0	3.2
	C( <u>O</u> )O	531.0	27.9	2.0
	C-O	531.8	44.2	2.0
	C(O) <u>O</u>	533.5	27.9	2.0
Hydrogenated graphite powder annealed at 500 °C	Total O1s	531.9	100.0	2.9
	C( <u>O</u> )O	531.0	21.9	2.0
	C-O	532.0	56.2	2.0
	C(O) <u>O</u>	533.6	21.9	2.0