Electronic Supplementary Material (ESI) for Materials Advances.

A compared experimental and theoretical study of the mechanism of graphene oxide mild reduction by ascorbic acid and N-acetyl cysteine for biomedical applications

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ELECTRONIC SUPPLEMENTARY MATERIAL

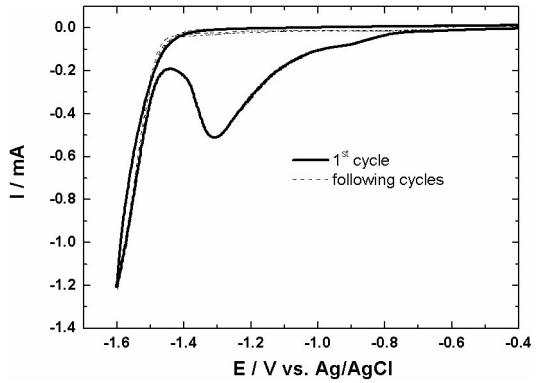

Figure S1. CV of **GO** drop casted onto GCE. Measurements were run in 1.0 M pH=7.2 PBS buffer solution at 20 mV s^{-1} potential scan rate. 2nd and 3rd cycles are displayed with a dashed line.

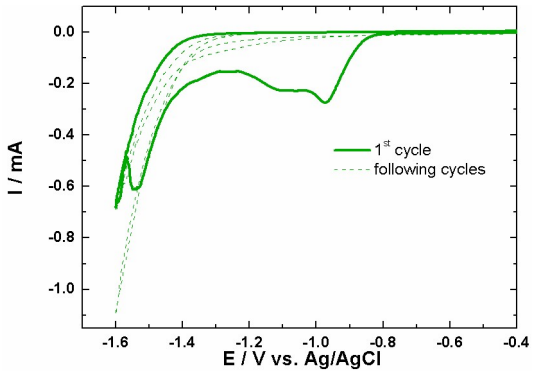

Figure S2. CV of **NAC 4h** m-rGO drop casted onto GCE. Measurements were run in 1.0 M pH=7.2 PBS buffer solution at 20 mV s^{-1} potential scan rate. 2nd and 3rd cycles are displayed with a dashed line.

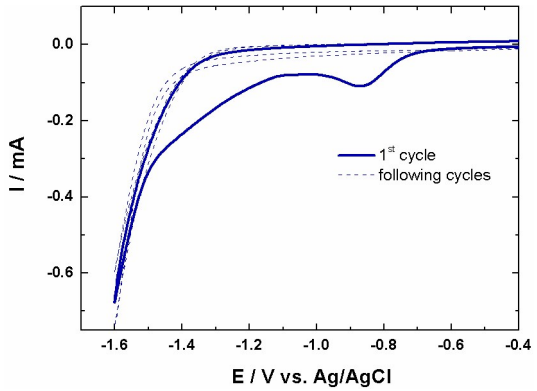

Figure S3. CV of **NAC 24h** m-rGO drop casted onto GCE. Measurements were run in 1.0 M pH=7.2 PBS buffer solution at 20 mV s^{-1} potential scan rate. 2nd and 3rd cycles are displayed with a dashed line.

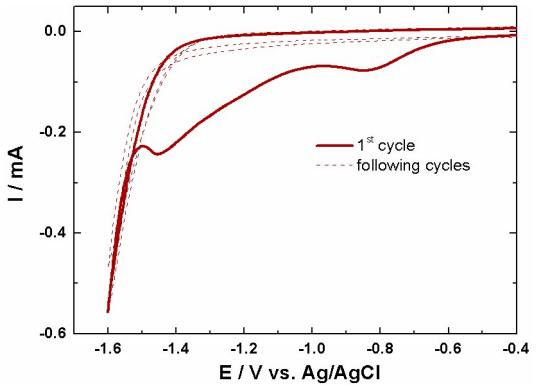

Figure S4. CV of **NAC 72h** m-rGO drop casted onto GCE. Measurements were run in 1.0 M pH=7.2 PBS buffer solution at 20 mV s^{-1} potential scan rate. 2nd and 3rd cycles are displayed with a dashed line.

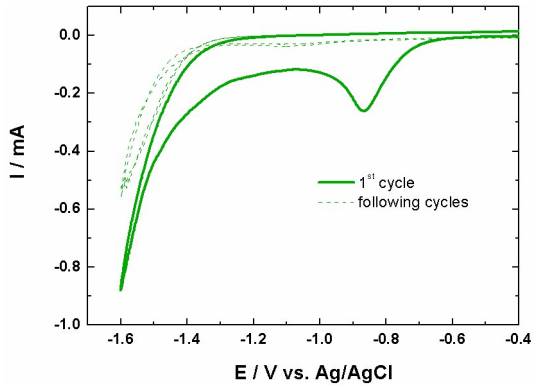

Figure S5. CV of **H_2A 4h** m-rGO drop casted onto GCE. Measurements were run in 1.0 M pH=7.2 PBS buffer solution at 20 mV s^{-1} potential scan rate. 2nd and 3rd cycles are displayed with a dashed line.

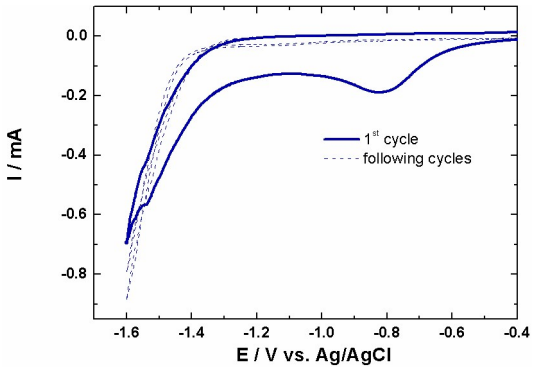

Figure S6. CV of **H_2A 24h** m-rGO drop casted onto GCE. Measurements were run in 1.0 M pH=7.2 PBS buffer solution at 20 mV s^{-1} potential scan rate. 2nd and 3rd cycles are displayed with a dashed line.

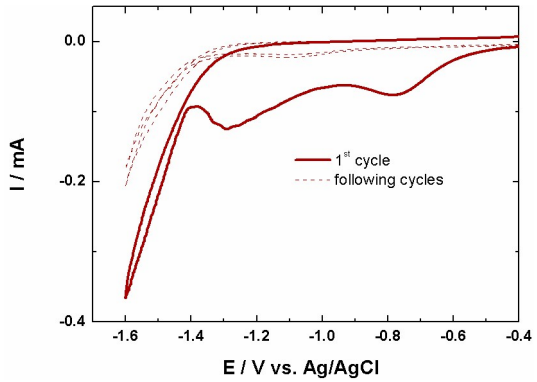

Figure S7. CV of **H_2A 48h** m-rGO drop casted onto GCE. Measurements were run in 1.0 M pH=7.2 PBS buffer solution at 20 mV s^{-1} potential scan rate. 2nd and 3rd cycles are displayed with a dashed line.

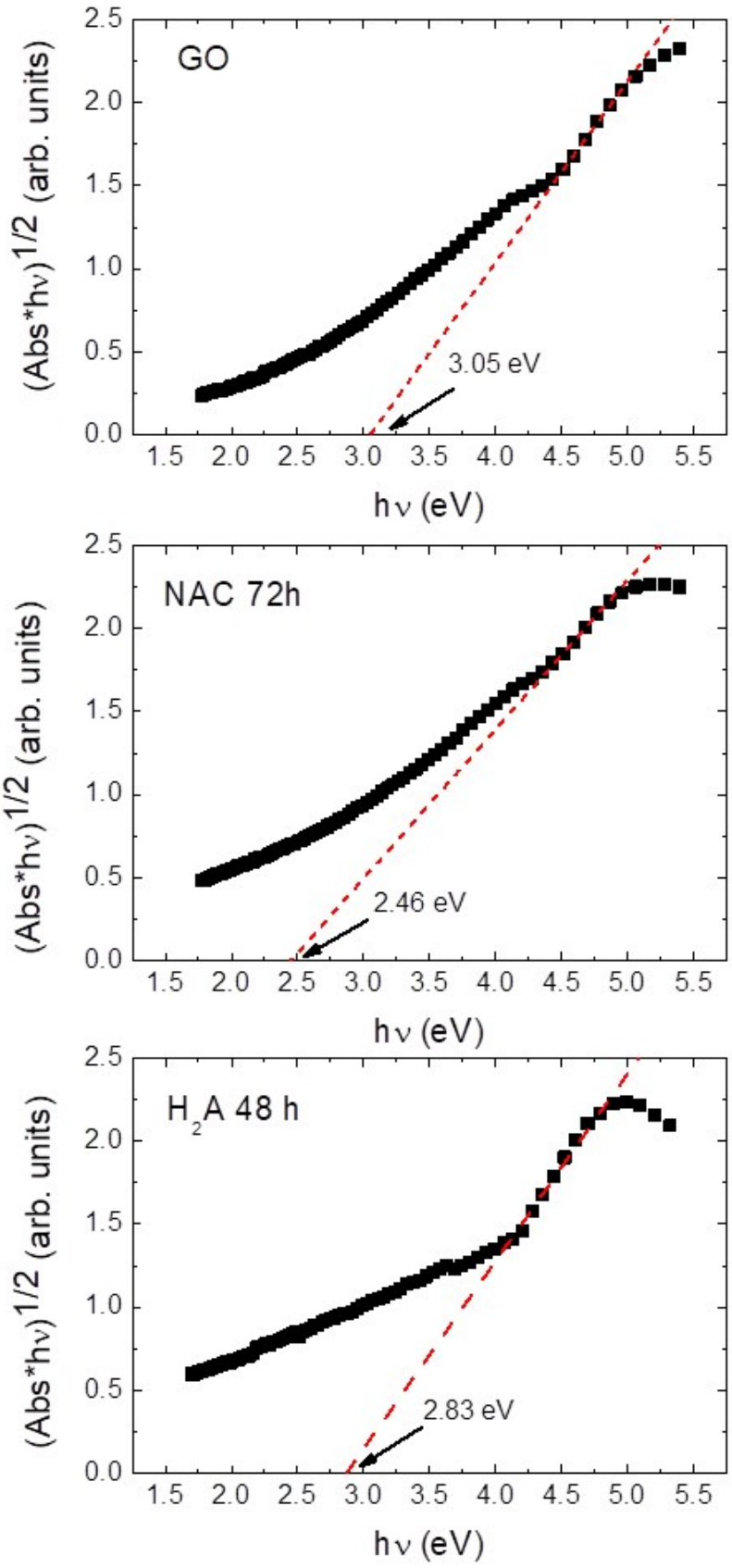

Figure S8. Tauc plots calculated from the absorption spectra to estimate the bandgap values of GO, NAC 72h and H_2A 48 h, as indicated.

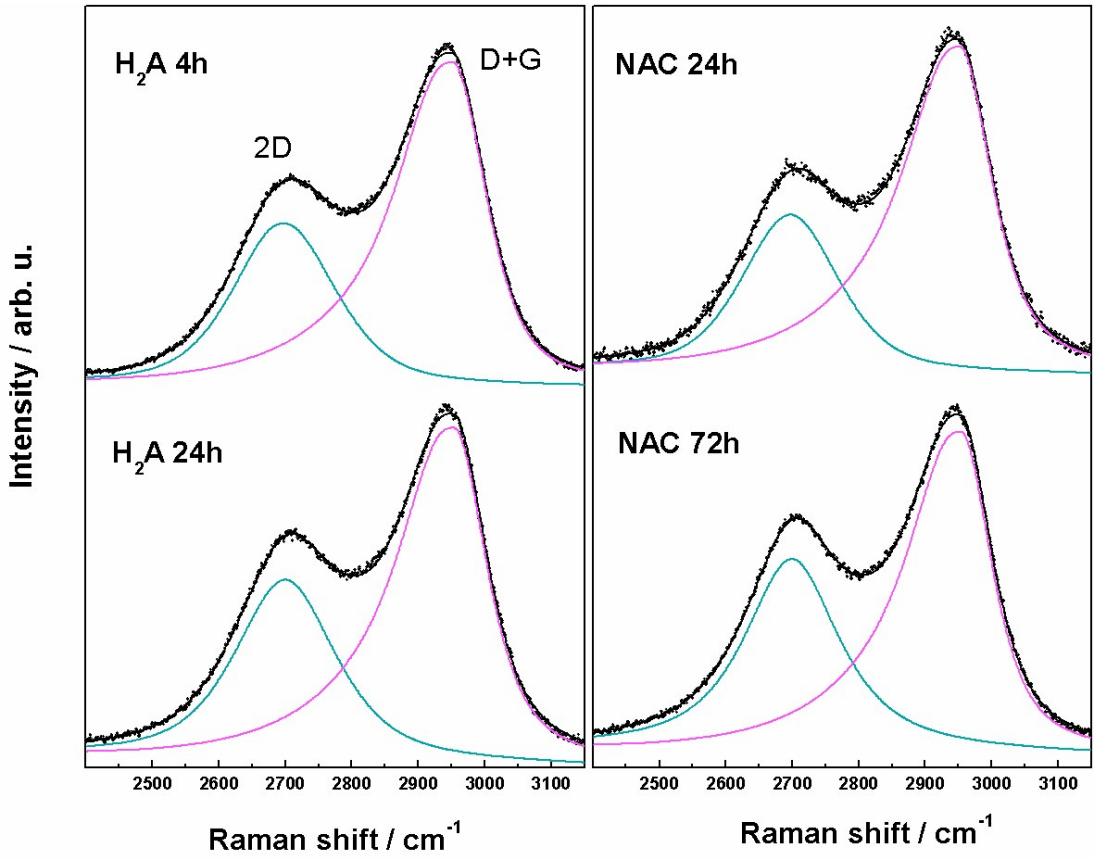

Figure S9. Raman spectra in the high wavenumber region of m-rGO samples: H_2A 4h, H_2A 24h, NAC 24h and NAC 72h. Experimental data (dots) have been fitted with symmetric and asymmetric Lorentzian model curves (continuous lines), associated to 2D (dark cyan) and D+G (magenta) peaks.

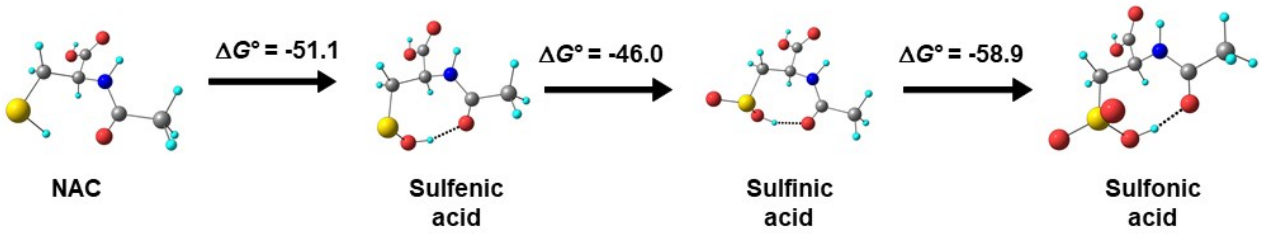

Figure S10. Sequential oxidation of NAC during successive reduction steps of epoxyl groups in GO. Reaction free Gibbs energy (kcal/mol) values are also reported.

Table S1. Electrochemical parameters associated to the reduction processes and resulting LUMO energy values for the samples addressed in this work.

sample	U_{onset} (V)	U_{peak} (V)	Q (C)	E_{LUMO} (eV)
GO	-0.923	-1.311	0.152	-4.03
NAC 4h	-0.862	-0.975	0.121	-4.09
NAC 24h	-0.713	-0.866	0.064	-4.24
NAC 72h	-0.593	-0.836	0.045	-4.36
H_2A 4h	-0.722	-0.869	0.070	-4.23
H_2A 24h	-0.582	-0.817	0.063	-4.37
H_2A 48h	-0.552	-0.774	0.025	-4.40

Table S2. Experimental values of Raman shift (cm^{-1}) and FWHM (cm^{-1}) of high wavenumber peaks (2D and D+G) in Raman spectra of selected samples addressed in this work.

	Raman shift (cm^{-1})/ FWHM (cm^{-1})	
sample	**2D**	**D+G**
H_2A 4h	2700/182	2952/166
H_2A 24h	2700/180	2954/166
NAC 24h	2697/172	2952/166
NAC 72h	2699/172	2954/158
erGO[a]	2704/137	2954/122
GO[a]	2708/202	2942/164

[a] Data taken from ref[1]

References

(1) Marrani, A. G.; Coico, A. C.; Giacco, D.; Zanoni, R.; Scaramuzzo, F. A.; Schrebler, R.; Dini, D.; Bonomo, M.; Dalchiele, E. A. Integration of graphene onto silicon through electrochemical reduction of graphene oxide layers in non-aqueous medium. *Appl. Surf. Sci.* **2018**, *445*, 404–414.