Supporting Information

Role of the carbon defects in the catalytic oxygen reduction by graphite nanoparticles: a spectromagnetic, electrochemical and modellistic integrated approach.

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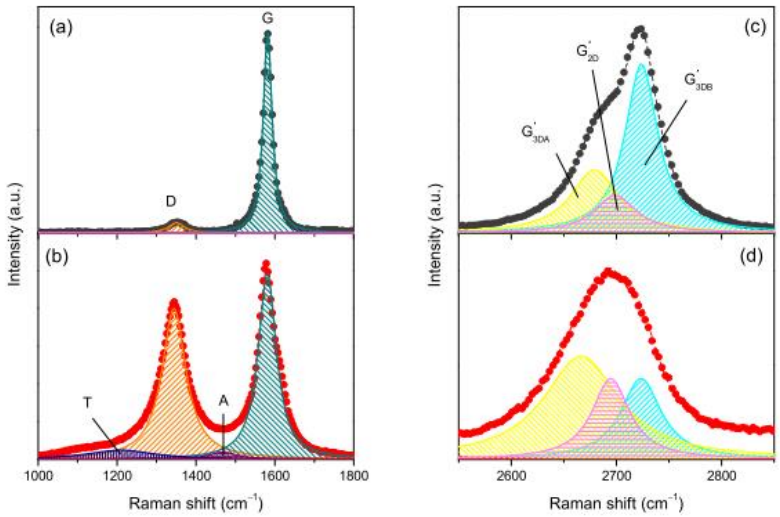

Figure S1. Results of spectra fitting. (a–b) First- and (c–d) second-order regions of the spectra of (a,c) commercial and (b,d) ball-milled graphites.

Table S1. Centre wavenumber positions (ω) and widths (γ, namely FWHM) of the main bands. The D/G and 3DB/(3DB+2D) integrated intensity ratios (I_D/I_G and $I_{3DB}/(I_{3DB}+I_{2D})$) are also reported.

Sample Code	ω_T (cm^{-1})	γ_T (cm^{-1})	ω_D (cm^{-1})	γ_D (cm^{-1})	ω_A (cm^{-1})	γ_A (cm^{-1})	ω_G (cm^{-1})	γ_G (cm^{-1})	I_D/I_G	$I_{3DB}/(I_{3DB}+I_{2D})$
PG			1352	46			1582	22	0.09	0.78
BM	1204	212	1344	75	1470	95	1581	55	1.08	0.37

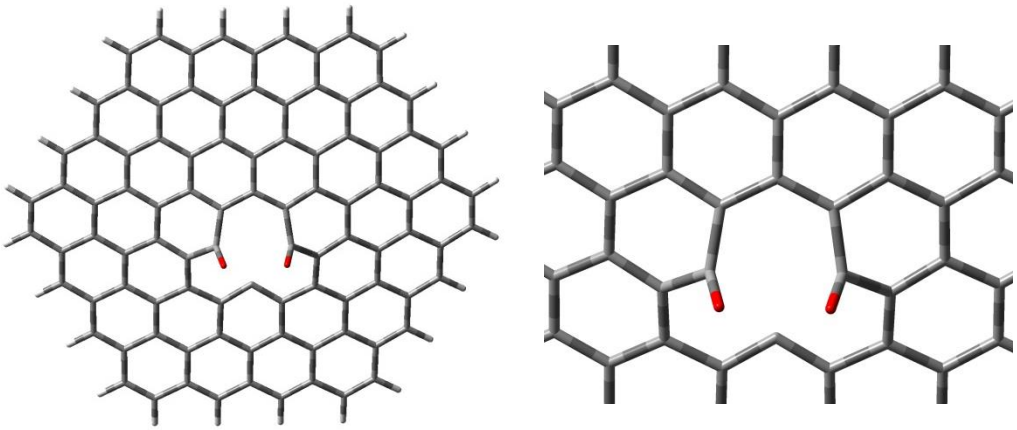

Figure S2. Reaction product of $C_{95}H_{24}$ with molecular oxygen

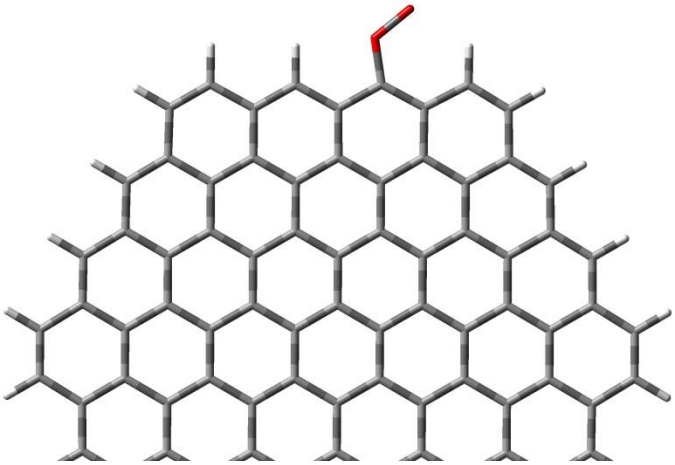

Figure S3. Reaction product of $C_{96}H_{23}$ with molecular oxygen

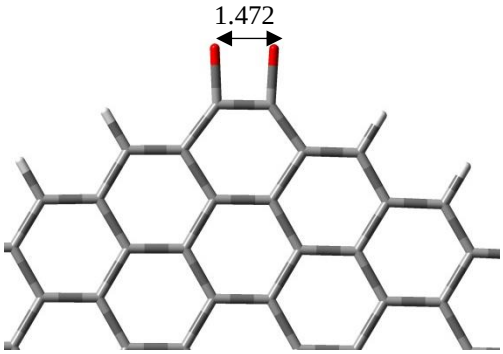

Figure S4. Reaction product of $C_{96}H_{22}$ with molecular oxygen

Table S2. Spin densities at the zig-zag and arm-chair positions of the considered $PAH^{(-)}$. In the case of $C_{150}H_{30}^{(-)}$, values at the $C^{(a)}$ and the $C^{(b)}$ zig-zag positions are reported (see text).

	$C_{24}H_{12}^{(-)}$	$C_{54}H_{18}^{(-)}$	$C_{96}H_{24}^{(-)}$	$C_{150}H_{30}^{(-)}$
Zig-zag	-	0.17	0.16	$C^{(a)}$ 0.20 $C^{(b)}$ 0.10 - 0.15
Arm-chair	0.20	0.04	0.02	0.01-0.06