SUPPLEMENTARY INFORMATION

Table S1. Properties of carbon-based materials modified with catalytic organic compounds for ORR towards H_2O_2 production.

Matrix	*Modifier*	*Eletrolyte*	*% (w/w)[a]*	*$\Delta E_{1/2}$ (mV)[b]*	*$\%H_2O_2$*	*Ref.*
PL6C	Sudan Red 7B	0.1 M K_2SO_4	0.5	~50	86.2	[1]
	methyl-p-benzoquinone	"	0.5	~20	85.5	[1]
	anthraflavic acid	"	0.5	~10	83.3	[1]
	anthraquinone-2-carboxylic acid	"	2.0	~0	83.8	[1]
	tert-butyl-anthraquinone	0.1 M K_2SO_4 0.1 M H_2SO_4	1.0	~50	89.6	[2]
	1,2-dihydroxyanthraquinone	"	1.0	~0	95.0	[3]
	2-methyl-1,4-naphthoquinone	"	0.5	~80	75.0	[3]
	acenaphthylene-1,2-dione	"	1.0	~20	84.0	[3]
	2-ethylanthraquinone	"	10	~400	*	[4]
GC	Azobenzene	0.1 M K_2SO_4 0.1 M H_2SO_4 (pH 1.0)	10	~300	*	[5]
	Antraquinone	0.1 M KOH	*	~15	95-100	[6]
	2,6-diaminoanthraquinone	0,2 M NaCl	2.6	~380	*	[7]
GRA	5-hydroxy-1,4-naphthoquinone	0.5 M CHCOONa	*	~160	*	[8]

a- Percentage of the modifier into the matrix in the weight / weight ratio

b- The values are calculated versus the reduction potential of unmodified electrode

***-** Unspecified values

Table S2. Experimental and theoretical values of dipole moment (in Debye, D) for 1,4-naphtoquinone in benzene, using B3LYP, CAM-B3LYP, different basis sets and C-PCM method

B3LYP	Experimental Dipole Moment = 1.21 D	
Basis set	B3LYP	CAM-B3LYP
6-311G	1.82	1.69
6-311++G	1.97	1.83
6-311G(2d,2p)	1.53	**1.42**
6-311G(3d,3p)	1.54	1.43
6-311++G(2d,2p)	1.70	1.60
6-311++G(3d,3p)	1.68	1.58
cc-pvqz	1.65	1.54
cc-pvtz	1.60	1.50
def2-TZVPD	1.69	1.57

Table S3. Values of Laplacian of electron density ($\nabla^2\rho$) for the hydrogen bonds in structures 1 and 2

	BCPs	**$\nabla^2\rho$ (a.u.)**
Structure 1	H67 – O68	0.04
Structure 2	H85 – O79	0.16
Structure 3	H87 – O77	0.03

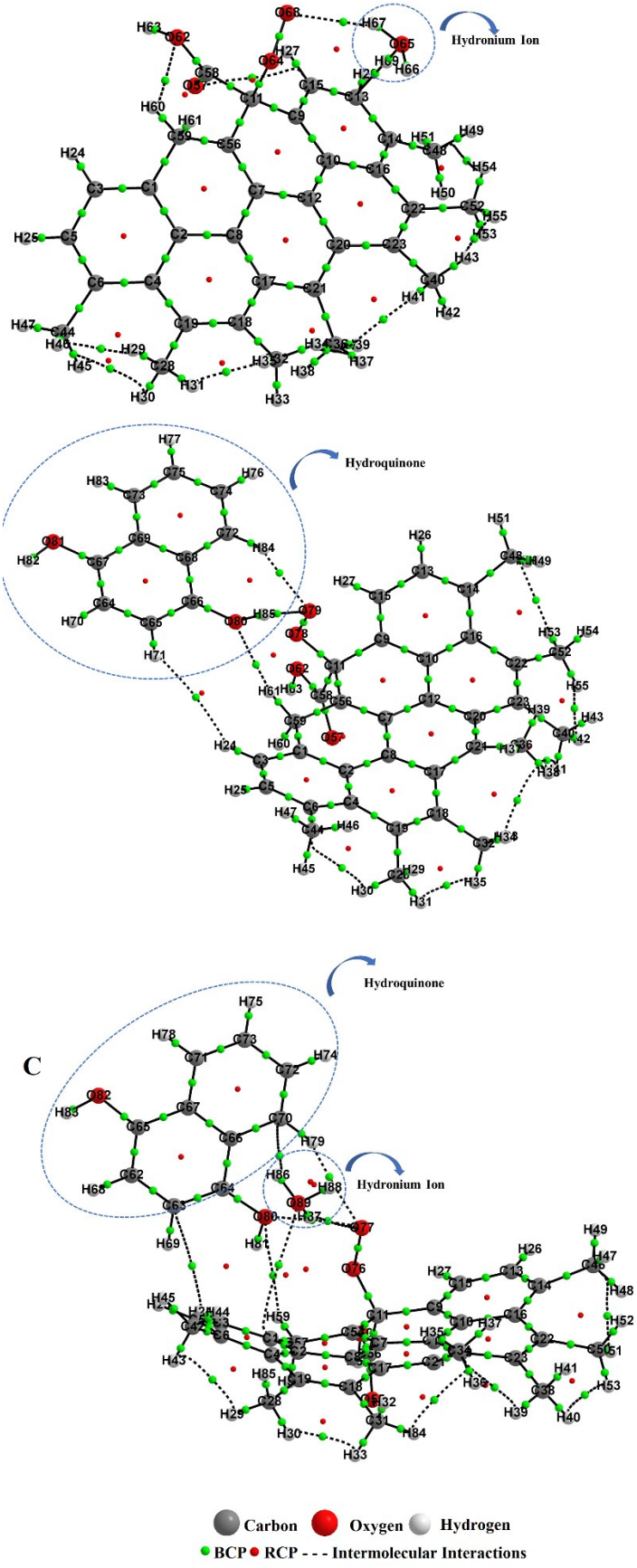

Figure S1. BCPs related to the Laplacian of electron density ($\nabla^2\rho$) for structures 1 (A), 2 (B) and 3 (C).

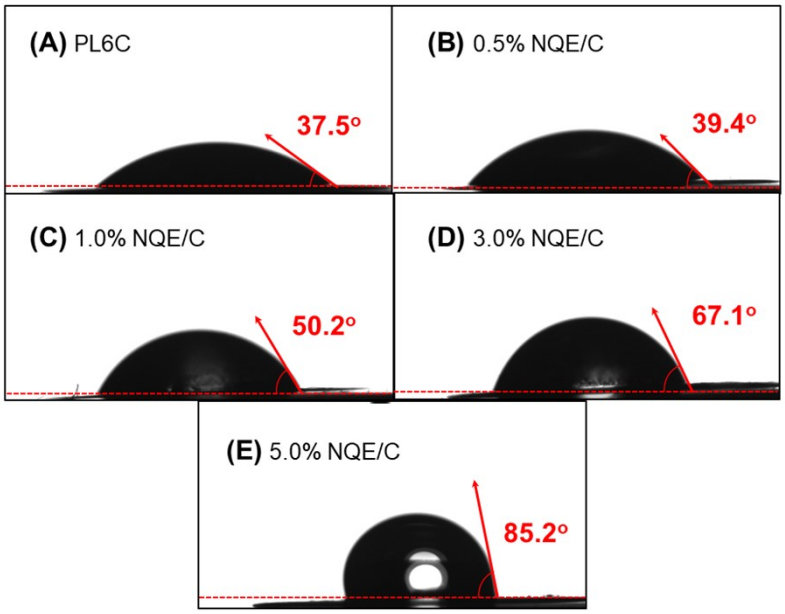

Figure S2. Pictures and contact angle measurements of a 3 µL ultrapure water drop on microlayers of PL6C **(A)**, 0.5% NQE/C **(B)**, 1.0% NQE/C **(C)**, 3.0% NQE/C **(D)** e 5.0% NQE/C **(E)**.

Table S4. Kinetic velocity of H_2O_2 electrogeneration from ORR in acid medium under the different current densities investigated

k_{app} values (mg L^{-1} min^{-1})						
Current density	***10 mA cm^{-2}***	***25 mA cm^{-2}***	***50 mA cm^{-2}***	***75 mA cm^{-2}***	***100 mA cm^{-2}***	***150 mA cm^{-2}***
PL6C	0.595	1.410	3.419	4.477	4.595	4.426
1.0% NQE/C	0.657	1.514	4.126	5.302	4.871	4.944

Advanced Oxidative Process	**k_{app} (min^{-1}) 1.0% NQE-GDE**	**R^2 Curve**
UVC	0.3×10^{-3}	0.9973
AO	6.6×10^{-3}	0.9887
AO-H_2O_2	8.1×10^{-3}	0.9909
AO-H_2O_2/UVC	8.3×10^{-3}	0.9896
EF	11.4×10^{-3}	0.9709
PEF	16.4×10^{-3}	0.9761

Table S5. Kinetic constant of PRM degradation calculated based on the different AOP applied in acid medium at j=75 mA cm^{-2}.

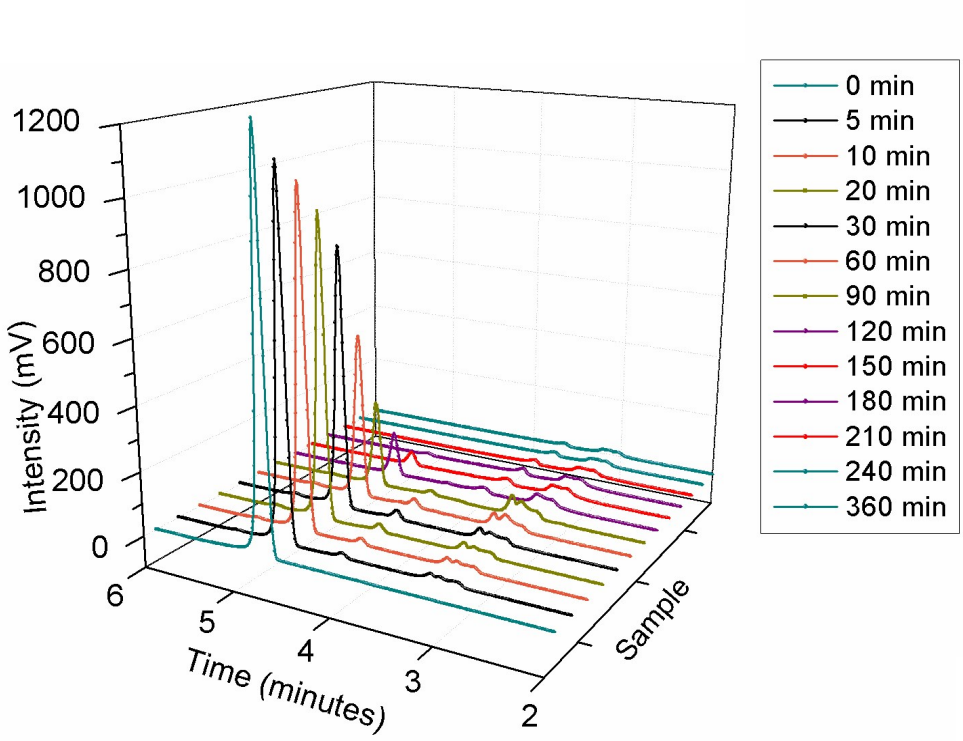

Figure S3. PRM chromatographic peaks related to 6 h of PEF degradation process conducted on 1.0 % NQE modified GDE using 0.1 mol L^{-1} K_2SO_4 under pH 2, with UVC light and 0.15 mmol L^{-1} of Fe^{2+}.

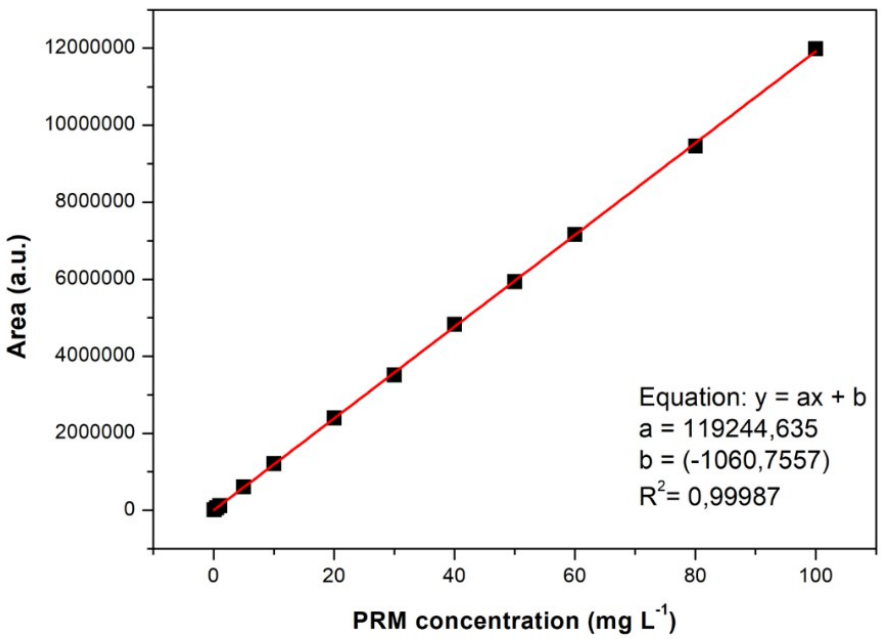

Figure S4. Paracetamol analytical curve developed by HPLC-UV using the external standard method in the concentration range of 0.5 to 100 mg L^{-1}.

References

1 J. Moreira, V. Bocalon Lima, L. Athie Goulart and M. R. V. Lanza, *Appl. Catal. B Environ.*, 2019, **248**, 95–107.

2 R. B. Valim, R. M. Reis, P. S. Castro, A. S. Lima, R. S. Rocha, M. Bertotti and M. R. V Lanza, *Carbon N. Y.*, 2013, **61**, 236–244.

3 R. S. Rocha, R. B. Valim, L. C. Trevelin, J. R. Steter, J. F. Carneiro, J. C. Forti, R. Bertazzoli and M. R. V. Lanza, *Electrocatalysis*, 2020, **11**, 338–346.

4 J. C. Forti, R. S. Rocha, M. R. V. Lanza and R. Bertazzoli, *J. Electroanal. Chem.*, 2007, **601**, 63–67.

5 J. C. Forti, J. A. Nunes, M. R. V. Lanza and R. Bertazzoli, *J. Appl. Electrochem.*, 2007, **37**, 527–532.

6 A. Sarapuu, K. Vaik, D. J. Schiffrin and K. Tammeveski, *J. Electroanal. Chem.*, 2003, **541**, 23–29.

7 L. Roullier, E. Waldner and E. Laviron, *J. Electroanal. Chem.*, 1985, **191**, 59–73.

8 M. C. Pham and J. E. Dubois, *J. Electroanal. Chem.*, 1986, **199**, 153–164.