Electronic Supplementary Material (ESI) for Green Chemistry.

Supplementary Information

Electro Fenton's Reaction Coupled Zn-Air Battery for In-Situ Pollutant Degradation

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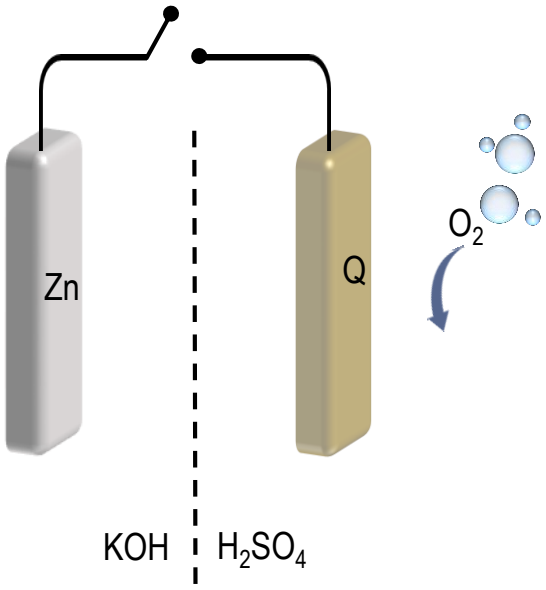


Scheme S1. Schematic representation of the battery architectural components.

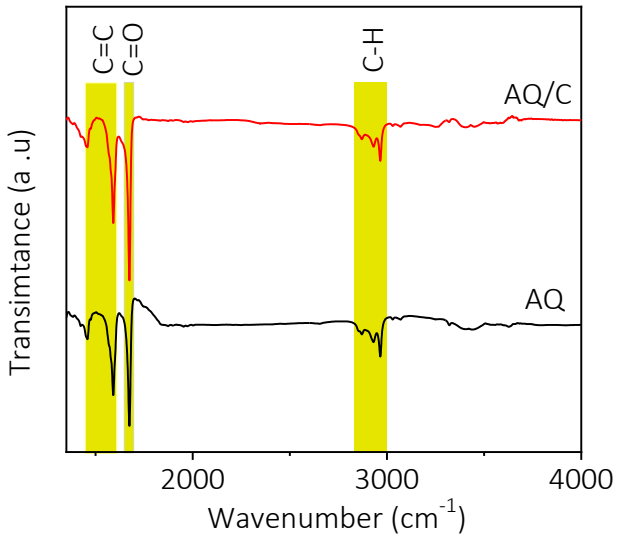


Figure S1. FTIR spectra of AQ and AQ/C composite materials.

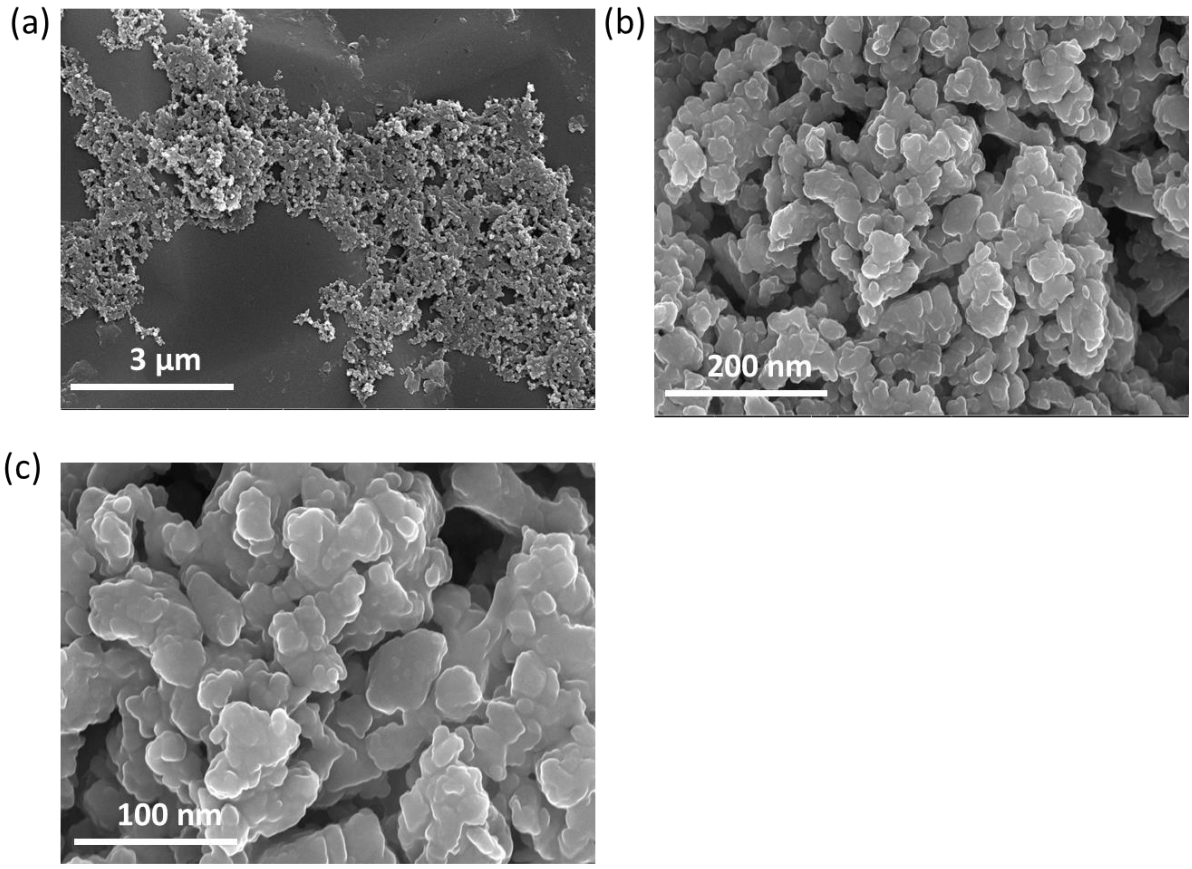


Figure S2. FESEM images of the AQ/C composite at different magnifications.

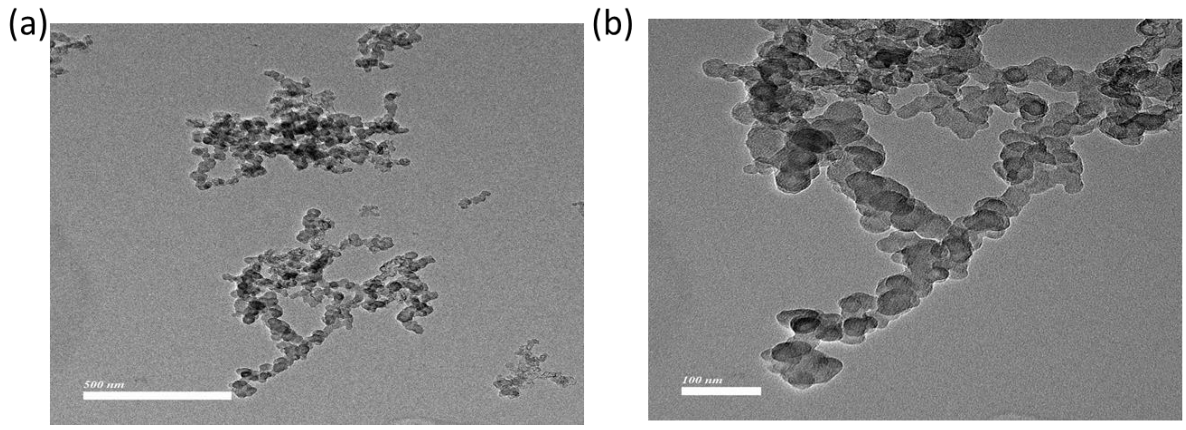
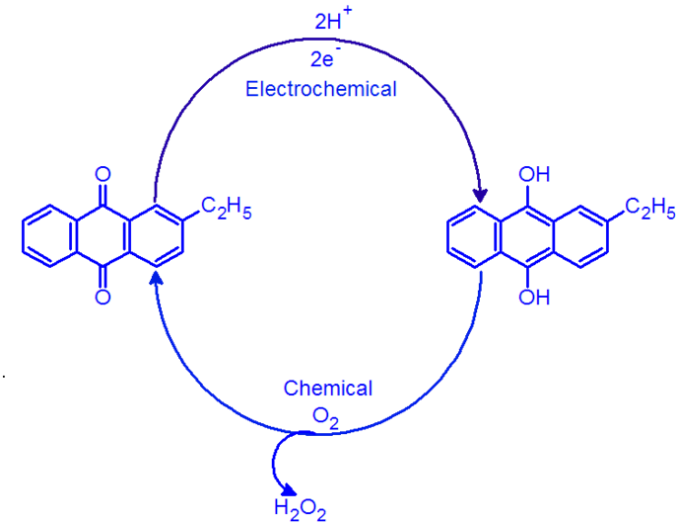


Figure S3. HRTEM images AQ/C composites at (a, b) different magnifications.



Scheme S2. Reaction scheme for the electrochemical reduction of ethylanthraquinone and its chemical oxidation in presence of O_2 to generate H_2O_2. [Ref: 1, 2]

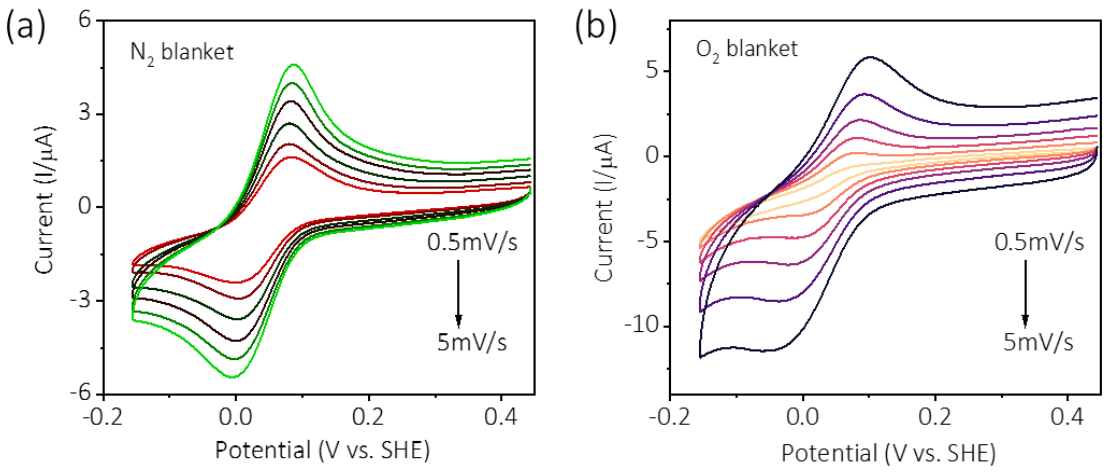


Figure S4. Cyclic voltammograms of AQ/C electrode at different scan rates in 0.5 M H_2SO_4 solution in (a) N_2saturated solution and (b) oxygen saturated solution.

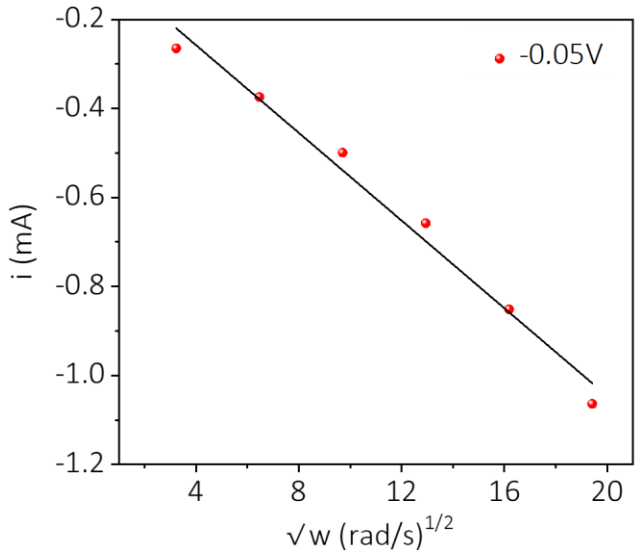


Figure S5. Levich plot extracted from Figure 1e.

Calculation S1.

Finding the number of electrons using Levich equation

$1/\text{ slope} = 0.62\, n\, F\, A\, D^{(2/3)}\, u^{(-1/6)}\, C$

where,

F = 96485.33 C/mol

A = 0.196 cm^2

D = 1.93 $x10^{-5} cm^2/s$

Kinematic viscocity (u) = 0.0100

C = 1.26 $x10^{-6}$ M/cm^2

The Slope values were extracted from the Levich plot at 1600 RPM

at -0.05 V=4.9298 e^{-5},

at -0.1 V = 5.1148 e^{-5},

at -0.15 V = 5.5341 e^{-5} and

at -0.2 V = 6.0313 e^{-5}

Potential E(V) vs. SHE	**No. of electrons from RRDE**
-0.05 V	2.15
-0.1 V	2.23
-0.15 V	2.41
-0.2 V	2.63

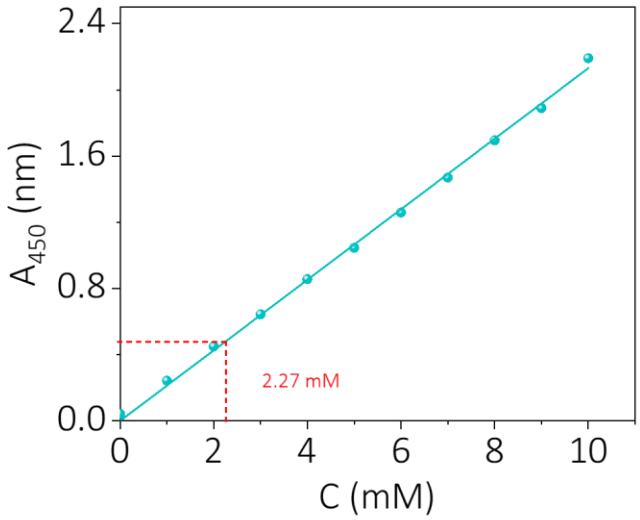


Figure S6. Calibration plot extracted from Figure 2d.

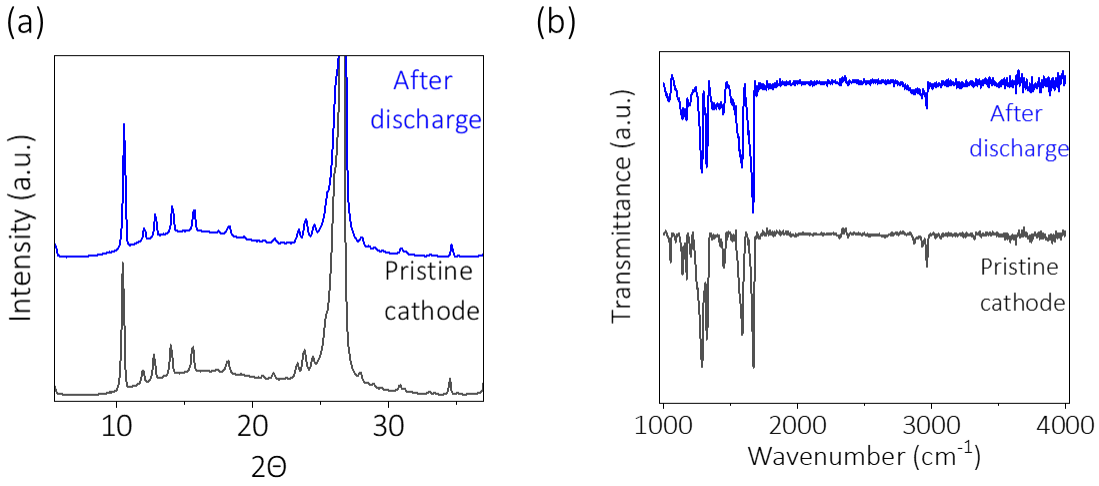


Figure S7. (a) XRD and (b) FTIR spectra of AQ/C composite electrode before and after battery discharge.

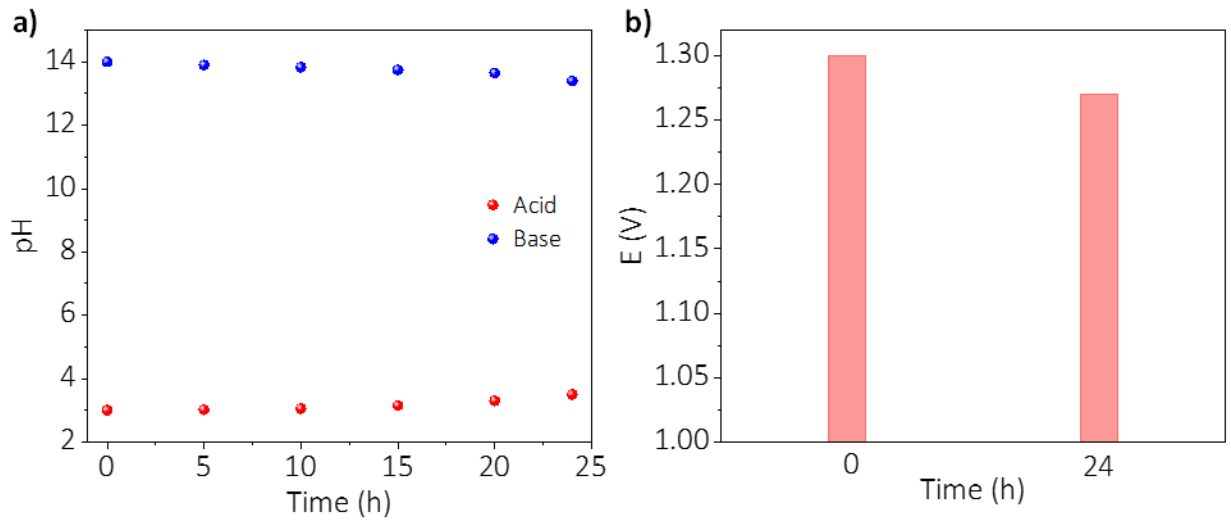


Figure S8. (a) pH of anodic and cathodic half-cells under open circuit condition (OCV) for a period of 24 hours. (b) OCV at t = 0 hr and t = 24 hr.

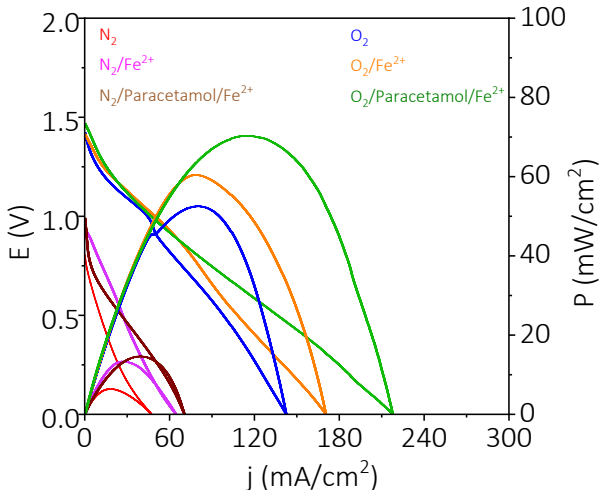


Figure S9. Polarization curves of the Zn-air battery at varying conditions (with and without Fe^{2+}/ paracetamol / purging with N_2 or O_2).

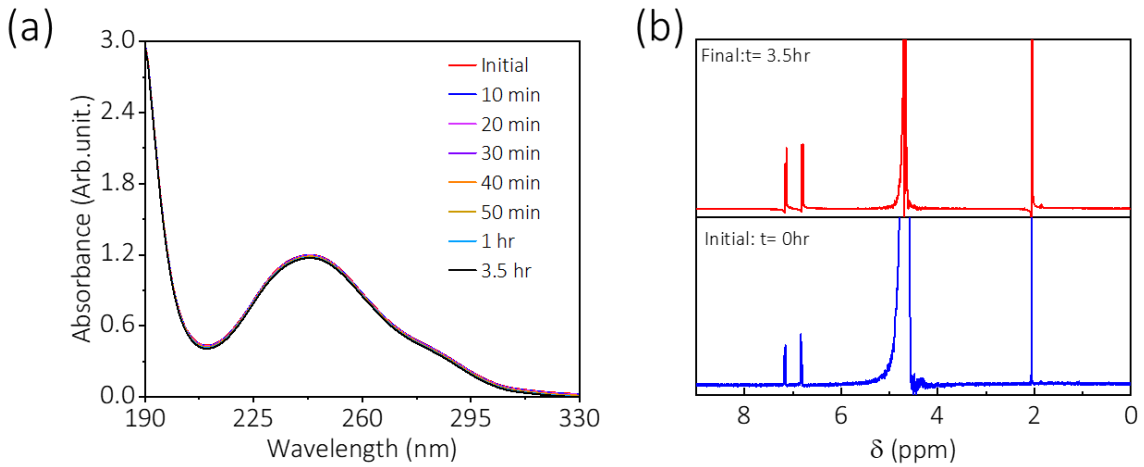
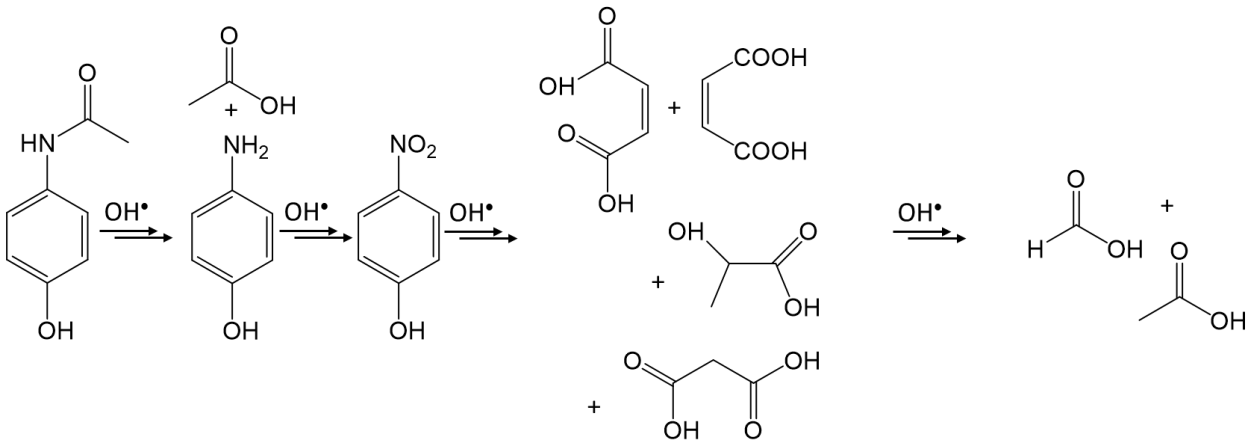


Figure S10. (a) Time dependent UV-Vis spectra of the battery catholyte in absence of Fe^{2+} ions. (b) NMR spectra of the catholyte before and after the battery discharge in absence of Fe^{2+} ions.



Scheme S3. Schematic representation showing the hydroxyl radical assisted degradation pathways of paracetamol forming formic acid and acetic acid. [Ref: 3]

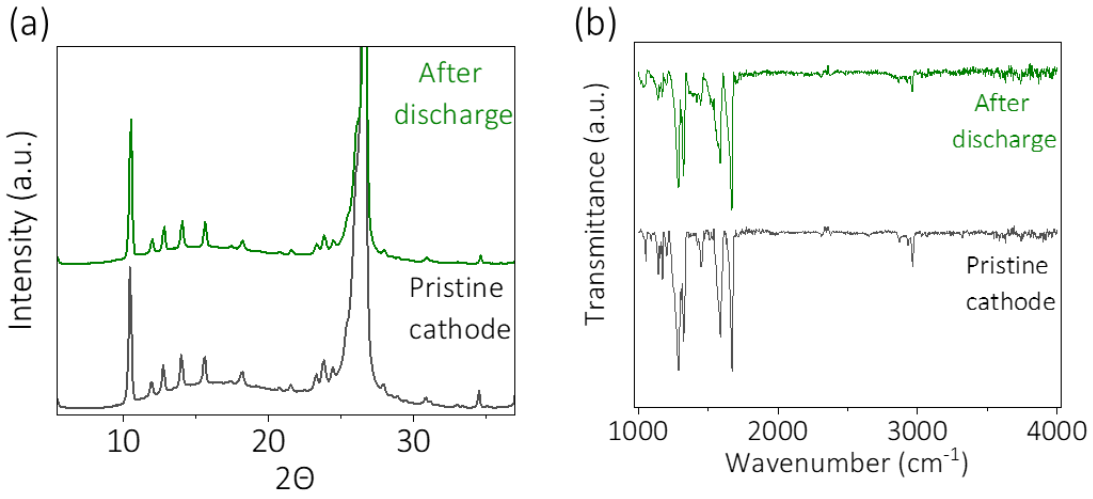


Figure S11. (a) XRD and (b) FTIR spectra of AQ/C composite electrode before and after battery discharge.

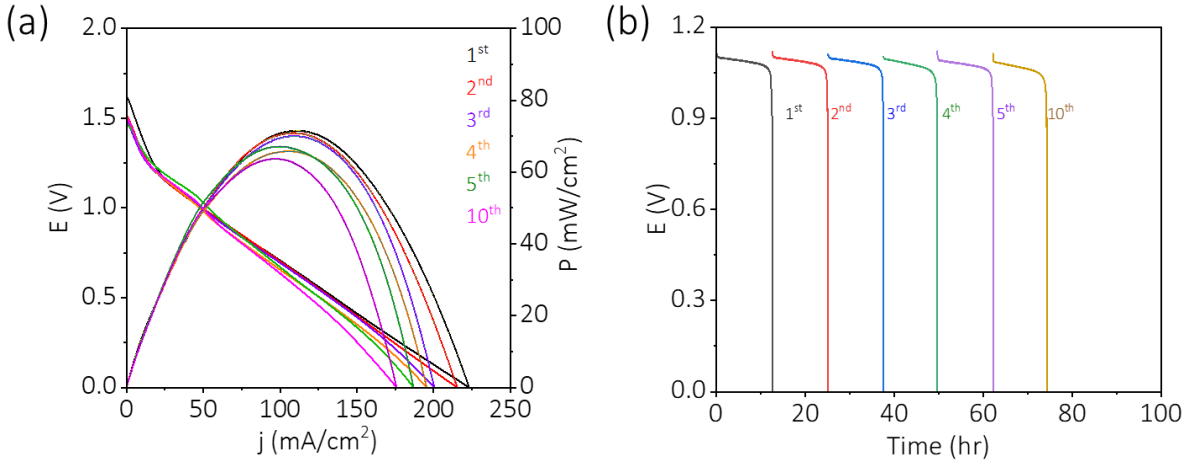
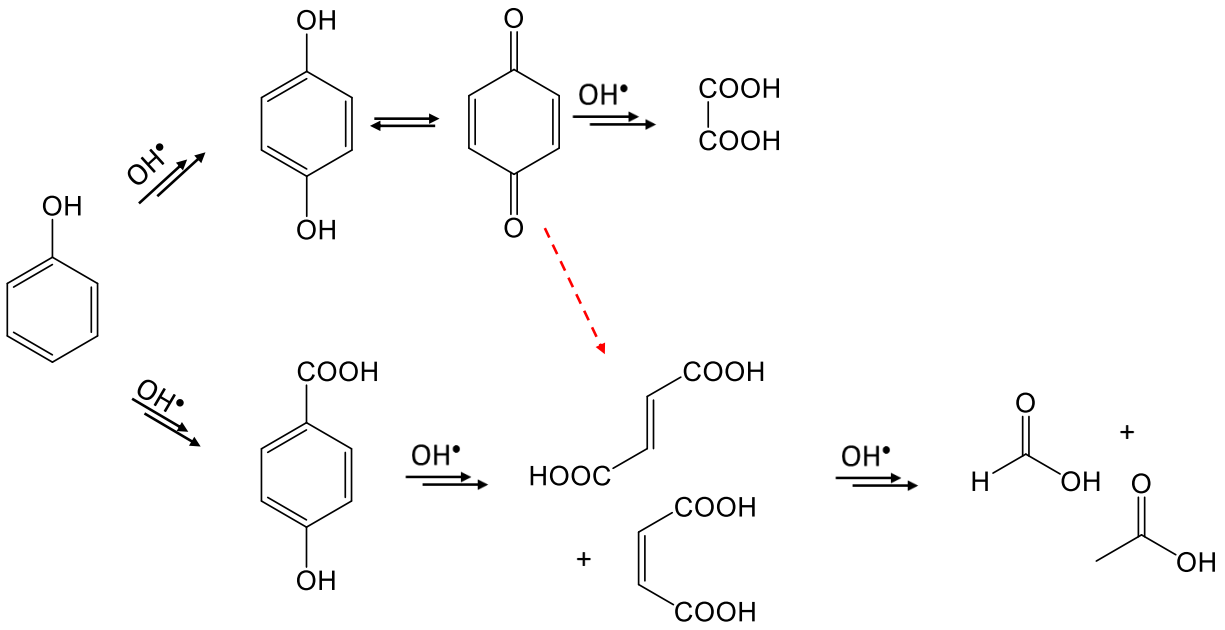


Figure S12. The performance of the pollutant degrading air battery for multiple cycles in O_2-purged H_2SO_4 solution (pH 3) containing 0.2 mM Fe^{2+} and paracetamol (0.5 mM). (a) Polarization curves of the Zn-air battery and (b) the corresponding galvanostatic polarization at 10 mA/cm^2.



Scheme S4. Schematic representation showing the hydroxyl radical assisted degradation pathways of phenol forming formic acid and acetic acid. [Ref: 4]

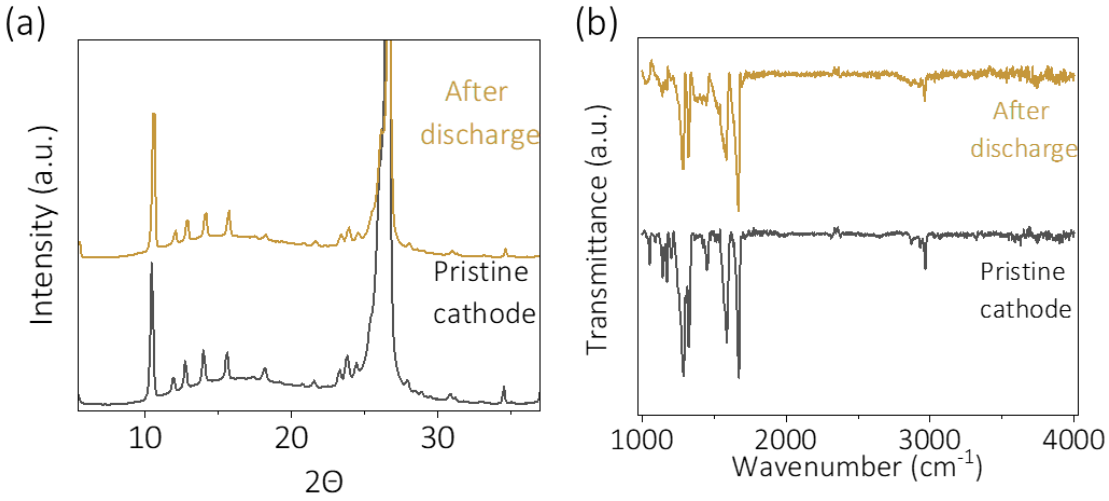


Figure S13. (a) XRD and (b) FTIR spectra of AQ/C electrode before and after battery discharge.

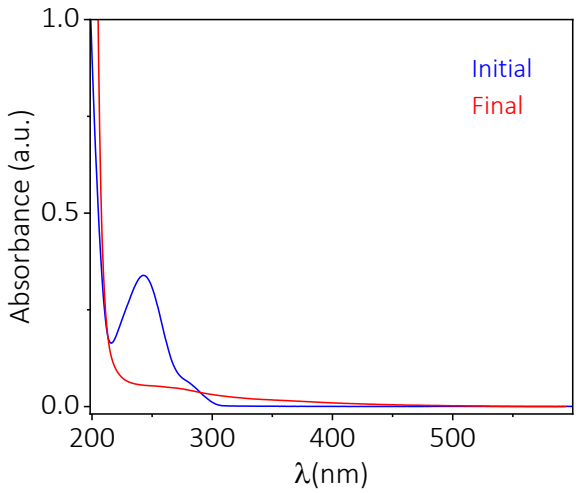


Figure S14. UV-Vis spectra of the electrolyte before and after discharge at 5 mA cm^{-2}.

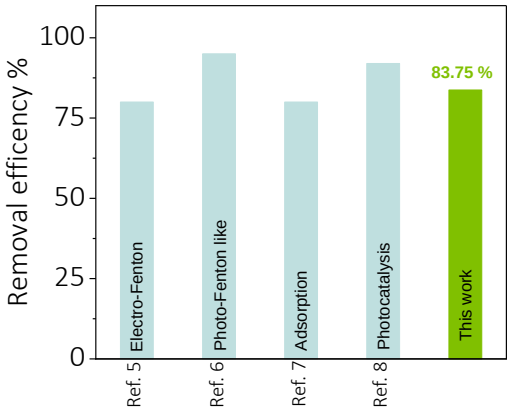


Figure S15. Degradation efficiency (%) demonstrated by various methods in comparison to this work.

References

1. J. M. Campos-Martin, G. Blanco-Brieva and J. L. G. Fierro, *Angew. Chemie Int. Ed.*, 2006, **45**, 6962–6984.
2. H. B. Vibbert, C. Bendel, J. R. Norton and A. J. Moment, *ACS Sustain. Chem. Eng.*, 2022, **10**, 11106–11116.
3. N. Villota, J. M. Lomas and L. M. Camarero, *J. Photochem. Photobiol. A Chem.*, 2016, **329**, 113–119.
4. G. Yang, H. Chen, H. Qin, X. Zhang and Y. Feng, *Can. J. Chem. Eng.*, 2017, **95**, 1518–1525.
5. X. Zheng, M. Gao, C. Liang, S. Wang and X. Wang, *Electrochim. Acta*, 2022, **428**, 140910.
6. A. Abdelhaleem, H. N. Abdelhamid, M. G. Ibrahim and W. Chu, *J. Clean. Prod.*, 2022, **379**, 134571.
7. G. Sivarasan, V. Manikandan, S. Periyasamy, M. S. AlSalhi, S. Devanesan, P. S. Murphin Kumar, R. rao Pasupuleti, X. Liu and H.-M. Lo, *Environ. Res.*, 2023, **227**, 115723.
8. M. Chijioke-Okere, A. H. Abdullah, Z. A. Mohd Hir, J. I. Alinnor and E. E. Oguzie, *Inorg. Chem. Commun.*, 2023, **148**, 110377.