**Supplementary data**

**Electrochemical degradation of 2,4-Dinitrotoluene (DNT) from aqueous solutions using three-dimensional electrocatalytic reactor (3DER): Degradation pathway, evaluation of toxicity and optimization using RSM-CCD**

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**Table S1.** 2,4- DNT chemical structure and its related information

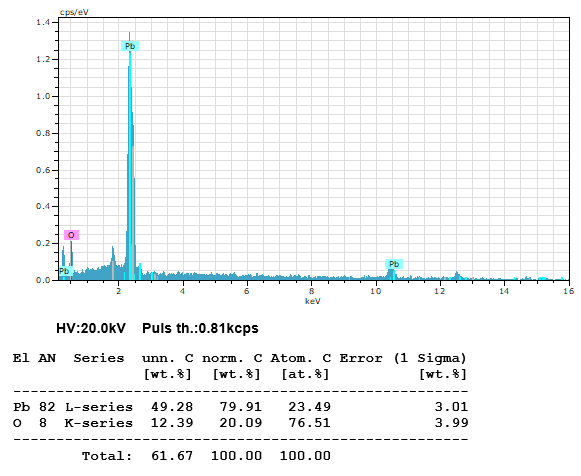
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| --- | --- |
| Component | Information/schematic/value |
| Chemical formula | C8H6Cl2O3 |
| structure | 2,4-dinitrotoluene - Kovats Retention Index |
| [Molar mass](https://en.wikipedia.org/wiki/Molar_mass) | 182.14 g/mol |
| [Melting point](https://en.wikipedia.org/wiki/Melting_point) | 70 °C (158 °F; 343 K) |
| [Boiling point](https://en.wikipedia.org/wiki/Boiling_point) | Decomposes at 250–300 °C |
| [Solubility in water](https://en.wikipedia.org/wiki/Aqueous_solution) | 270 mg/L at 22 °C |
| LD50 | 268 to 650 mg/kg (oral, rats)  1,954 mg/kg (oral, mouse)  1250 to 1954 mg/kg (oral, mice) |
| pKa in 298.15 k | 2.8 |
| Vapor pressure | 1.4 x 10-4 mm Hg at 22 ° C |

**Table S2**. Growth inhibition percentage in inlet and outlet solution by 3DER to remove 2,4-DNT under optimal conditions (2,4-DNT concentration = 23.5 mg/L, *j* = 4.8 mA/cm2, pH =4.1, electrolysis time= 50 min, GAC dose = 5 g/250cc))

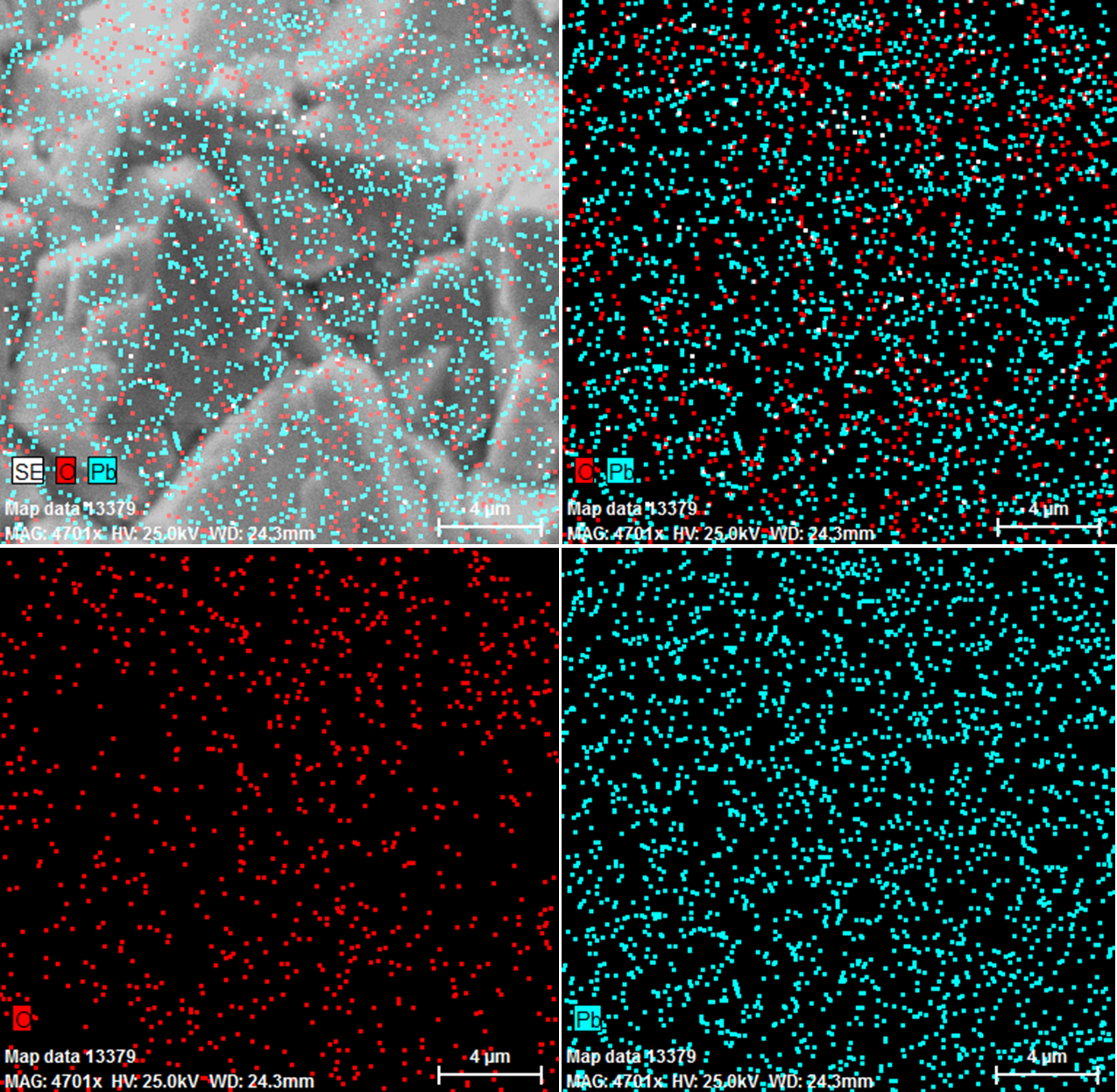
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| --- | --- | --- | --- | --- | --- | --- |
| Time (h) | Growth inhibition percentage of *Escherichia* | | | Growth inhibition percentage of *Staphylococcus aureus* | | |
| **Inlet** | **Outlet** | | **Inlet** | **Outlet** | |
| 2 | 75.8 | | 12.4 | 62.1 | | 18 |
| 4 | 65.9 | | 21.0.3 | 46.0 | | 14.0 |
| 6 | 47.9 | | 5.7 | 34.3 | | 12.5 |
| 8 | 46.4 | | 13.7 | 30.5 | | 10.6 |
| 10 | 42.4 | | 11.6 | 26.2 | | 7.83 |
| Average | 55.68 | | 10.85 | 39.82 | | 12.58 |

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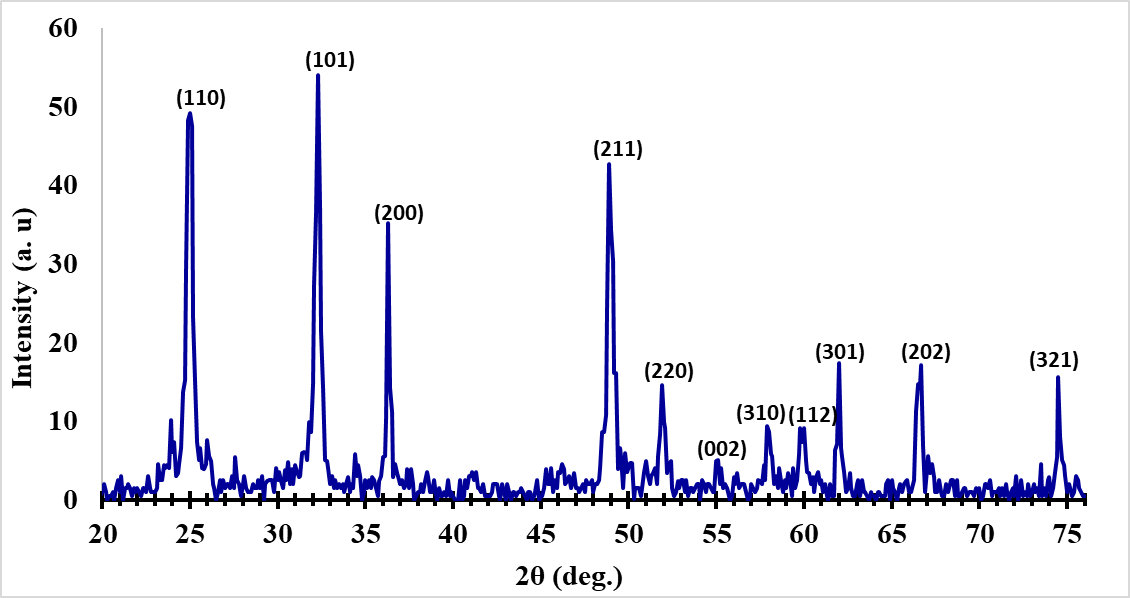
**Fig. S1.** FESEM images of the surface morphology at different magnifications of the β-PbO2 electrodeposited on graphite substrates.



**Fig. S2.** EDS spectrum of the G/β-PbO2 anode



**Fig. S3.** EDS mapping of the G/β-PbO2 anode

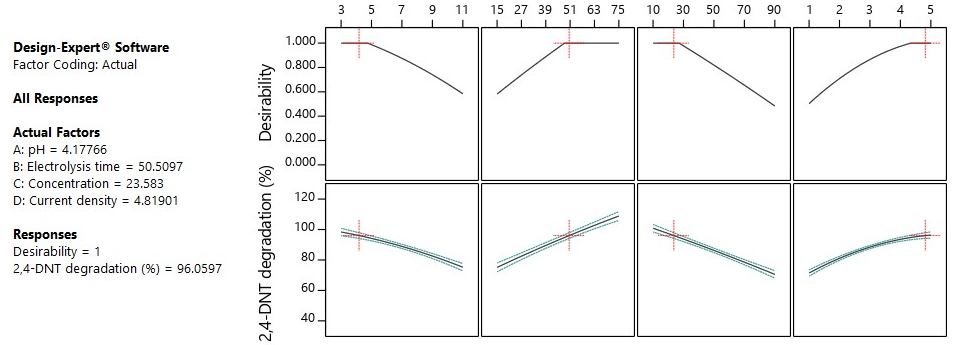


**Fig. S4.** XRD pattern of the G/β-PbO2 anode

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| (a) |
| (b) |

**Fig. S5.** (a) SEM image, and (b) XRD of MCZ@Fe3O4 nanoparticles

**Fig. S6.** Pareto chart of the main effects obtained from the screening experiments.



**Fig. S7.** Desirability ramp and the optimal points obtained by CCD for numerical optimization of four selected goals.

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**Fig. S8.** Reusability of G/β-PbO2 anode for electrodegradation of 2,4-DNT by 3DER (2,4-DNT concentration = 10.0 mg/L, Current density = 5.0 mA/cm2, pH =3.0, Electrolysis time = 75 min, GAC dose = 6 g/250cc)