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Supplementary Material for

Mechanistic investigation of the photocatalytic activity of PEDOT for aqueous contaminant removal: The role of iron and hydroxyl radicals

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Text S1. Hexazinone analysis

The residual concentrations of hexazinone were analyzed using LC-MS/MS (Shimadzu, Japan). The separation was done on a 2.1×100 mm, 3.5μ m, Eclipse Plus C18, Agilent column. The eluents consisted of 95% of 5 mM ammonium formate in water with 5% acetonitrile (mobile phase A) and 100% acetonitrile (mobile phase B). The tandem mass spectrometer was operated in a positive electrospray ionization mode (+ESI) over a mass scan range of m/z 40–600. The injection volume was two μ L, and the retention time was 7.6 min. The gradient program for hexazinone identification was performed at a flow rate of 0.2 mL/min and started with 100% A and 0% B. Then, the ratio was changed to 10% A and 90% B within 8 min. Within the next 2 min, the system returned to its initial conditions. The limit of detection (LOD) and the limit of quantification (LOQ) for hexazinone were estimated to be 0.2 and 0.8 μ g/L, respectively (Jasemizad and Padhye 2019).



Fig S1. Effect of Fe in the presence and absence of MeOH on photodegradation of MB exposed to UVC (experimental conditions: $[MB]_0$ = 15.6 μ M, [Fe (III)]_0= 0.05 mM, MeOH= 0.5 mM, pH~ 6.5).



Fig S2. Electrodeposition of PEDOT using (A) chronoamperometry mode with a potential of 1.1 V, and (B) CV mode with a potential range of 0.0 to 1.4 V from EDOT monomer solution (0.05 M) in 0.1 M LiClO₄ electrolyte solution in ACN.

The adsorption and desorption experiments were carried out for 15.6 μ M (5 mg L⁻¹) MB with 4 h adsorption followed by 24 h desorption. The results revealed that about 70% of the mass of MB was adsorbed onto PEDOT during 4 h. Only 20% of the mass of MB was desorbed from PEDOT into Milli-Q water after 3 h desorption experiments. After that, slight adsorption (10% mass of MB) was observed in 24 h. The sonication of the sample for 1 h in Milli-Q water showed only 18% mass of MB desorbed into the solution.



Fig S3. The adsorption and desorption of MB on the PEDOT strip (experimental conditions: $[MB]_0= 15$ mg/L, pH ~ 6.5).



Fig S4. The degradation of hexazinone using CF under irradiation at different pHs (experimental conditions: $[hexazinone]_0=5 \ \mu M$, UVC intensity= 20 mW cm⁻²).



Fig S5. The comparison between the efficiency of the immobilized C-PEDOT and E-PEDOT with similar size $(25 \times 40 \text{ mm})$ after 2 h.



Fig S6. Effect of iron on hexazinone removal efficiency in the presence of PEDOT in the dark and under irradiation (experimental conditions: [hexazinone]₀= 5 μ M, [Fe (III)]₀= 0.005 and 0.015 mM, pH~ 6.5, UVC intensity= 20 mW cm⁻²).



Fig. S7. The conversion of Fe (III) to Fe (II) in Milli-Q water and hexazinone solution in the presence of E-PEDOT (experimental conditions: [hexazinone]₀= 5 μ M, [Fe (III)]₀= 0.074 mM (Fe (III): hexazinone ratios= 15:1), reaction time= 1 h, pH~ 6.5, UVC intensity= 20 mW cm⁻²).



Fig S8. Effect of iron on hexazinone removal efficiency in the presence of PEDOT dipped in FeCl₃ in the dark and under irradiation (experimental conditions: [hexazinone]₀= 5 μ M, pH~ 6.5, UVC intensity= 20 mW cm⁻²). The amount of iron after the treatment was measured by MP-AES.

Reference

Jasemizad, T. and Padhye, L.P. (2019) Simultaneous analysis of betrixaban and hexazinone using liquid chromatography/tandem mass spectrometry in aqueous solutions. MethodsX 6, 1863-1870.