

ELECTRONIC SUPPLEMENTARY INFORMATION

Multifunctional Nb-Cu Nanostructured Materials as Potential Adsorbents and Oxidation Catalysts for Real Wastewater Decontamination

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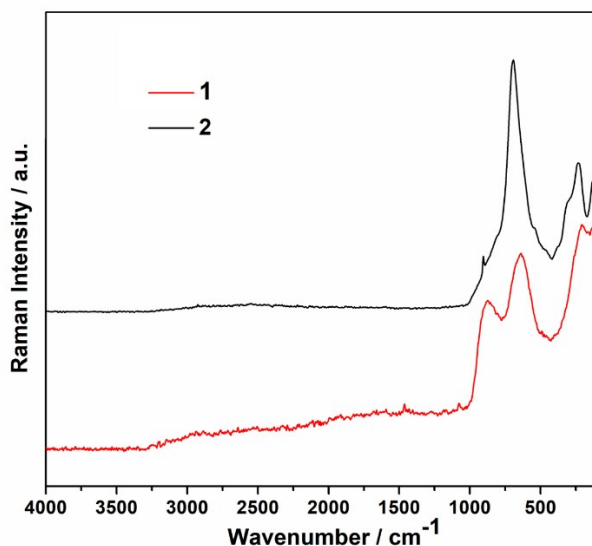


Fig. S1. Full-scale FT-Raman spectra of **1** (red line) and **2** (black line).

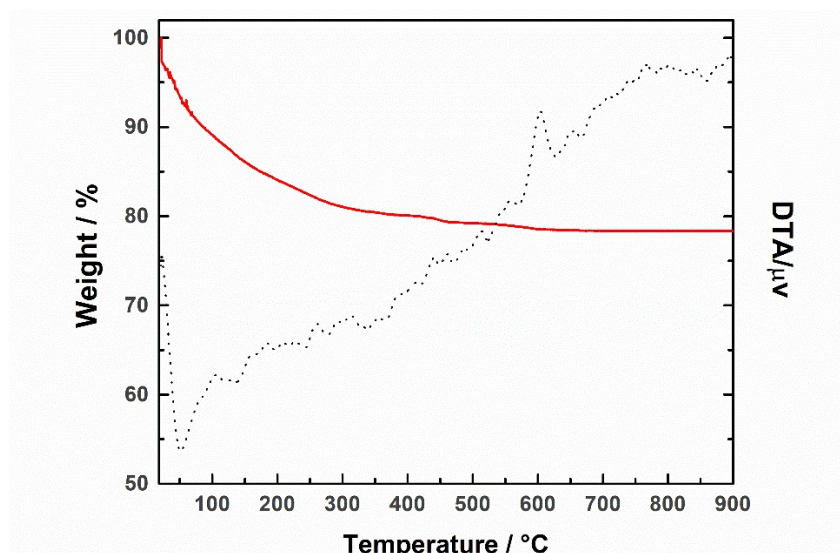


Fig. S2. TG (red line) and DTA (dashed black line) curves for **1**.

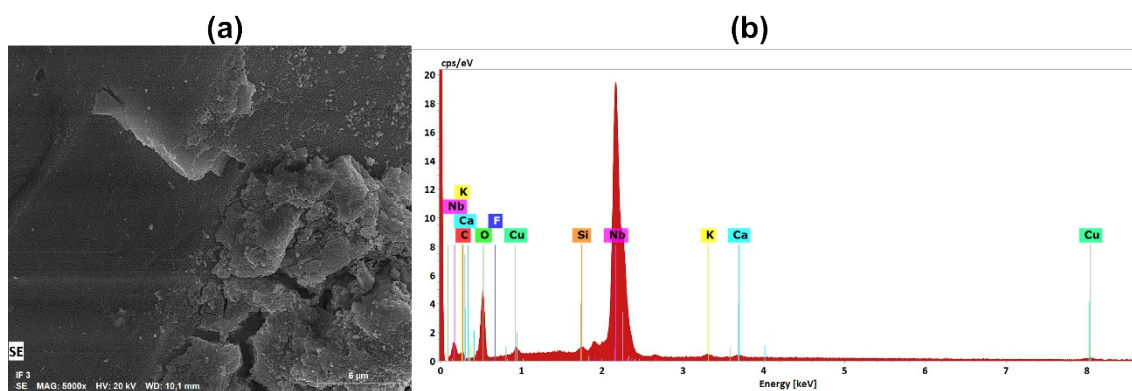


Fig. S3. Compilation of (a) SEM image (b)] with the EDS analysis for **1**.

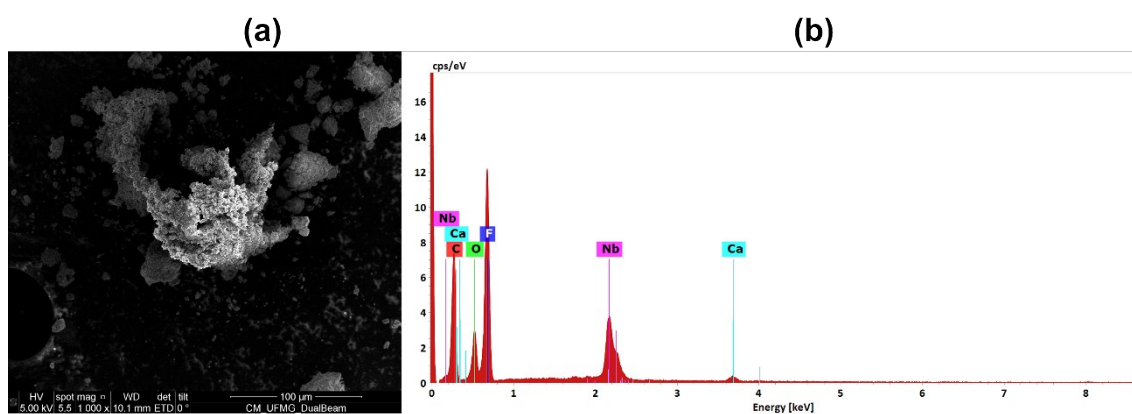


Fig. S4. Compilation of (a) SEM image (b)] with the EDS analysis for **2**.

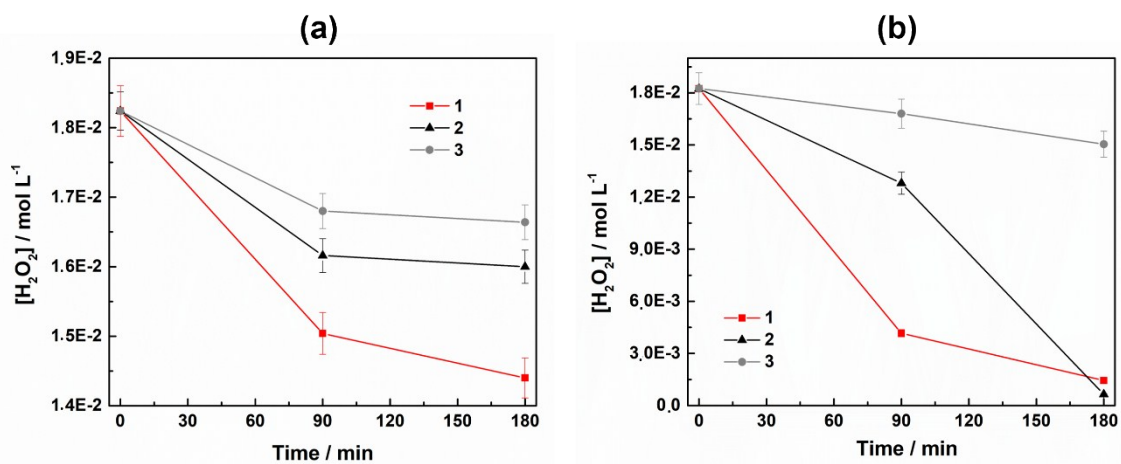


Fig. S5. Time-course H_2O_2 concentration determined by titration with permanganate in acidic medium [1,2] for Fenton-like reaction using materials **1-3** (a) in real wastewater contaminated MB and (b) ideal solution of MB. Both with $[\text{H}_2\text{O}_2]_0 = 1,84\text{E-}2 \pm 9.2\text{E-}4 \text{ mol L}^{-1}$.

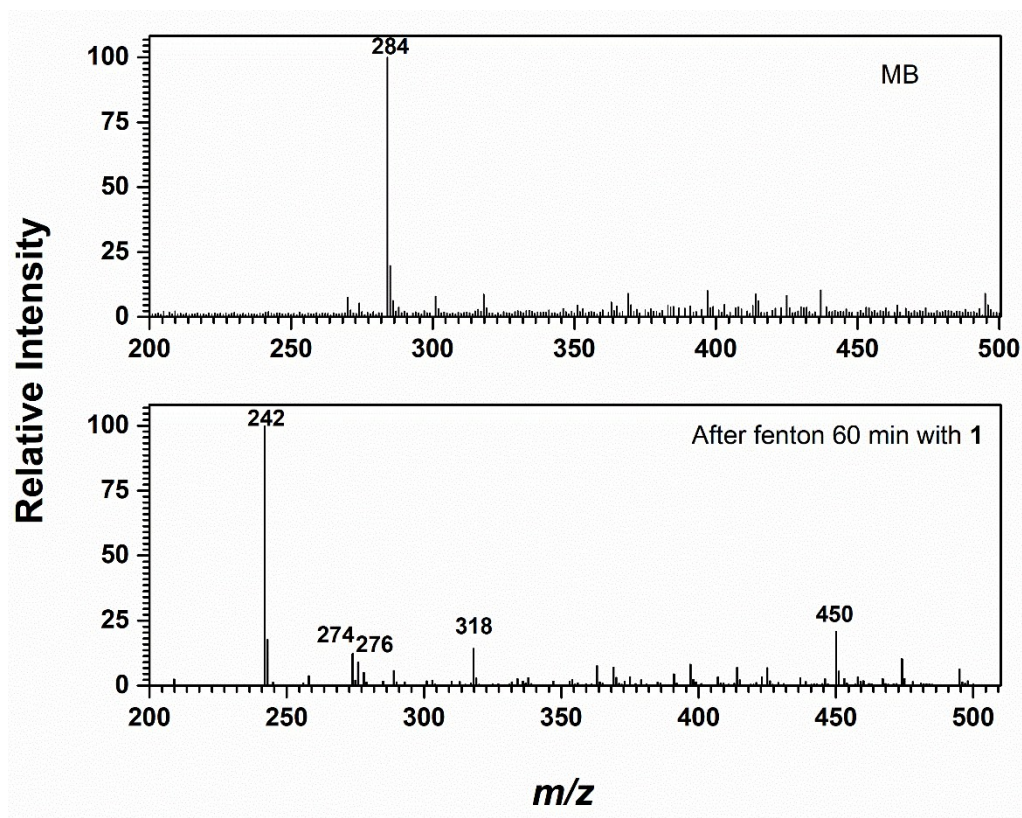


Fig. S6. ESI-MS(+) of MB dye and intermediates after the catalytic process for **1**.

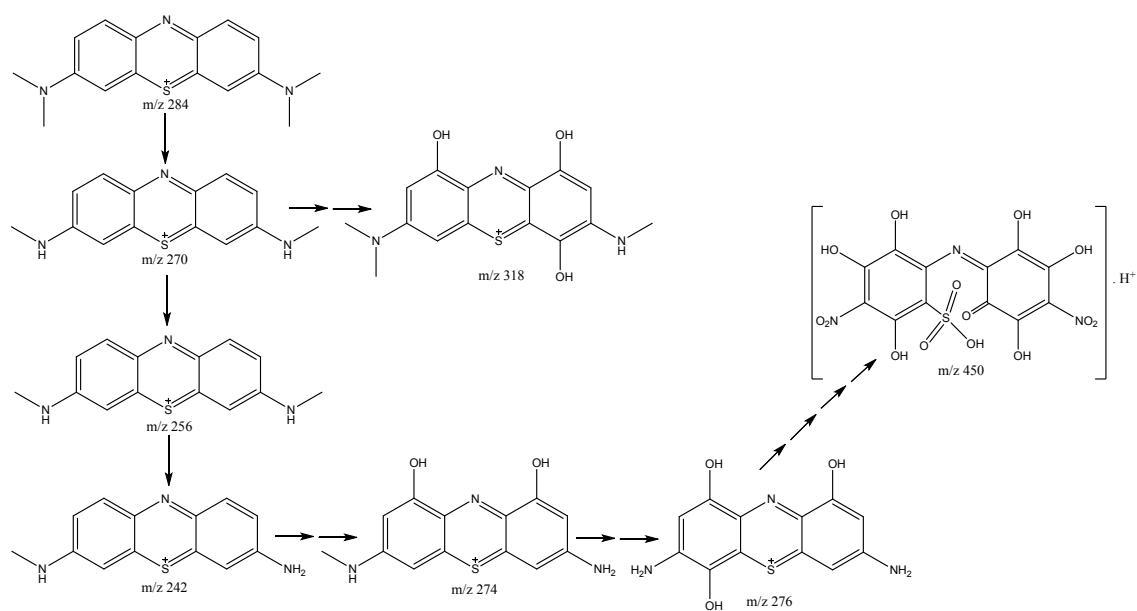


Fig. S7. Schematic representation MB dye intermediates observed by ESI-MS (+). These proposals were based on the literature and in our own attempts [3–5].

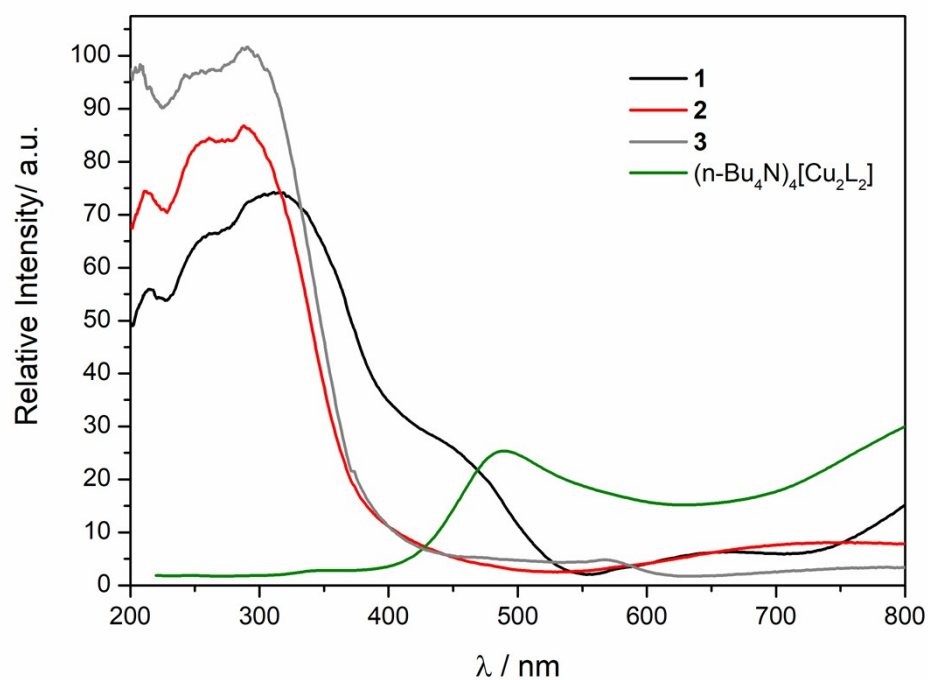


Figure S8. Diffuse reflectance UV-Vis spectra in solid for materials **1-3** and dicopper(II) complex $(n\text{-Bu}_4\text{N})_4[\text{Cu}_2\text{L}_2]$.

Table S1. Some physico-chemical parameters determined for water.

Solutions	T / °C	pH	OD (mg/L)	NO ₂ ⁻ (mg/L)
Control ⁱ	25.5±0.3 ^{a a}	7.3±0.2 ^a	6.200±0.105 ^a	0.0302±0.001 ^a
MB Real ⁱⁱ	25.0±0.7 ^a	7.1±0.2 ^a	5.800±0.208 ^a	0.0296±0.001 ^a
MB Real + Fenton ⁱⁱⁱ	24.8±0.2 ^a	7.2±0.4 ^a	6.400±0.238 ^a	0.0295±0.001 ^a
MB Real + Adsorption ^{iv}	24.1±0.3 ^a	7.6±0.2 ^a	6.600±0.397 ^a	0.0297±0.001 ^a

ⁱControl = distilled water; ⁱⁱMB Real = real effluent contaminated methylene blue; ⁱⁱⁱMB Real + Fenton = solution of real effluent contaminated methylene blue after Fenton reactions; ^{iv}MB Real + Adsorption = solution of real effluent contaminated with methylene blue after adsorption reaction. OD = Dissolved Oxygen. ^aThe mean values were expressed and compared to each other using GrapPad Prism software version 7.05. There was no statistical difference between the values found ($p > 0.05$). The parameters are within the reference values indicating good water quality for aquatic life (pH = 6 to 9.0, T = 24-26 degrees celsius, OD = above 4.0 mg /L and nitrite = lower to 1.0 mg /L - ABNT NBR15088 of 13-12-2016).

Table S2. Determination of Fe, Cu, Cr, Pb, Zn, Mg and Ca present in real effluent by atomic absorption analysis.

Effluent contaminated MB	ppm
Fe	0.852
Cu	<0.04*
Cr	<0.04*
Pb	0.297
Zn	0.148
Mg	1.897
Ca	21.330

*Below limit of detection (0.04 ppm for Cu and Cr)

Table S3. Total Organic Carbon (TOC) concentrations for effluent contaminated with MB and ideal solution of MB before and after Fenton-like reaction using material 1-2 for 180 min.

Sample	TOC/ mg L ⁻¹	(TOC/TOC ₀) x100
Effluent contaminated MB	172.081	
Effluent Contaminated MB – Fenton 180 min (1)	165.517	3.81%
Effluent Contaminated MB – Fenton 180 min (2)	167.172	2.85%
Ideal solution MB	3.613	
Ideal solution MB – Fenton 180 min (1)	3.452	4.45%
Ideal solution MB – Fenton 180 min (2)	3.172	12.20%

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