Supplementary Materials

Photocatalytic and Oxidative Synthetic Pathways for Highly Efficient PANI-TiO_2 Nanocomposites as Organic and Inorganic Pollutant Sorbents

Carolina Cionti [1,2], Cristina Della Pina [1,3], Daniela Meroni [1,2,*], Ermelinda Falletta [1,3,*] and Silvia Ardizzone [1,2]

[1] Dpt. of Chemistry, Università degli Studi di Milano, via Golgi 19, 20133 Milano, Italy.
[2] Consorzio INSTM, via Giusti 9, 50121 Florence, Italy.
[3] ISTM-CNR, via Golgi 19, 20133 Milano, Italy.
* Corresponding authors: daniela.meroni@unimi.it, ermelinda.falletta@unimi.it

Table S1. Composition of the adopted simulated drinking water.

Simulated Drinking Water	
Ca^{2+} (mg L^{-1})	45
Na^{+} (mg L^{-1})	46
Mg^{2+} (mg L^{-1})	9
Cl^{-} (mg L^{-1})	79
SO_4^{2-} (mg L^{-1})	37
HCO_3^{-} (mg L^{-1})	122
conductivity (µS cm^{-1})	478
pH	7.0

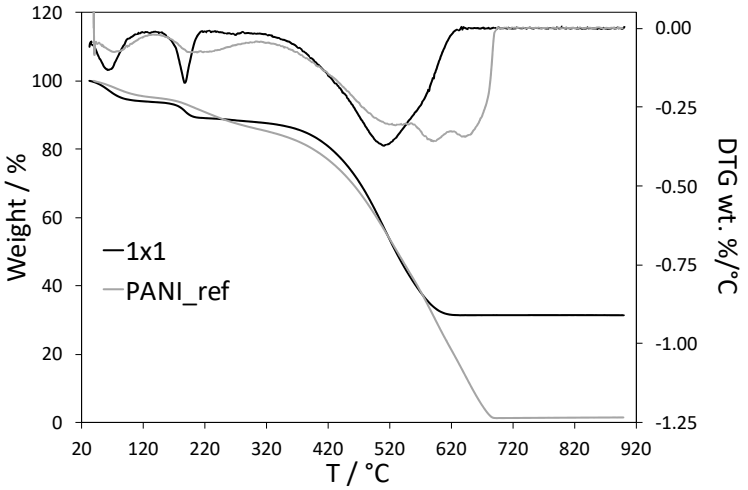


Figure S1. TGA and DTG analyses of 1 × 1 composite compared to reference PANI_ref.

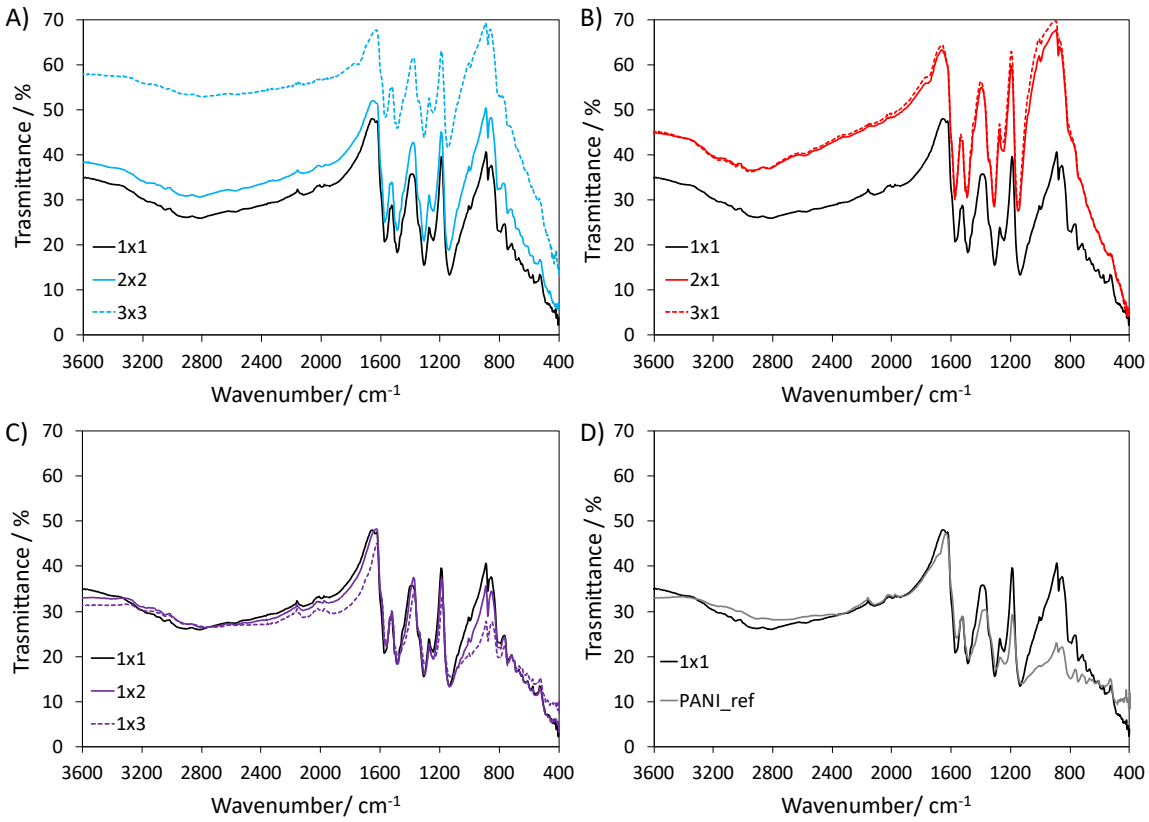


Figure S2. FTIR spectra of 1x1 composite compared to **A**) 2 × 2 and 3 × 3, **B**) 2 × 1 and 3 × 1, and **C**) 1 × 2 and 1x3, **D**) PANI_ref.

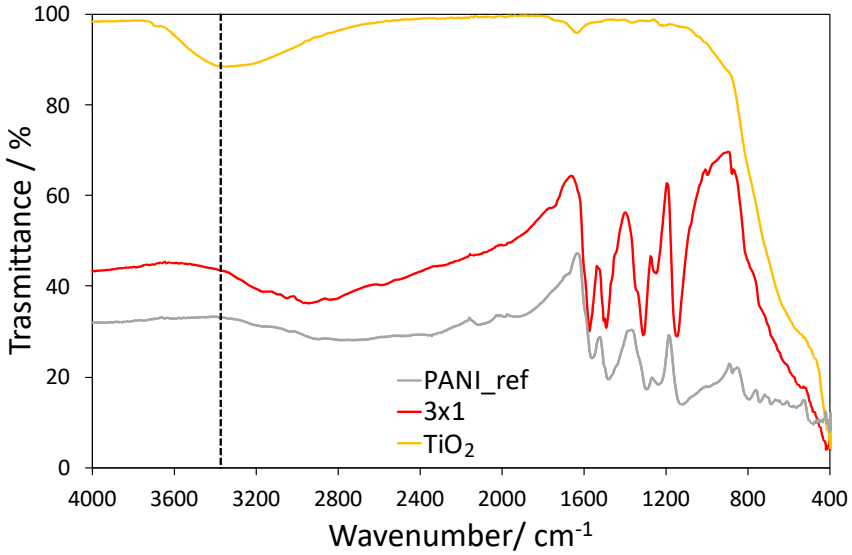


Figure S3. FTIR spectrum of 3 × 1 composite compared to those of PANI_ref and TiO_2: the vertical line is added only as a guide for the eyes.

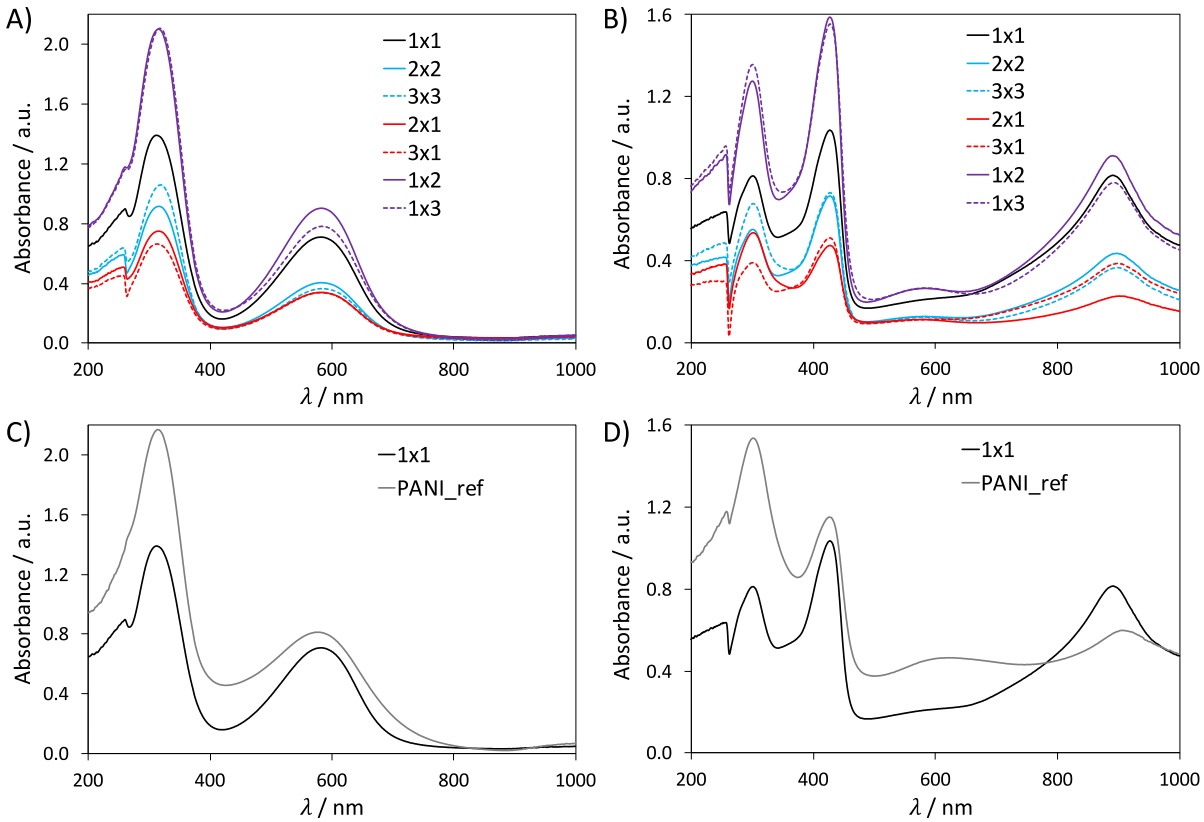
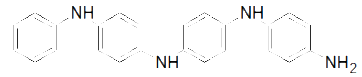
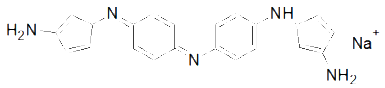
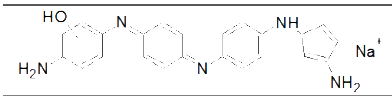
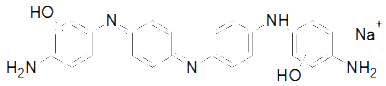
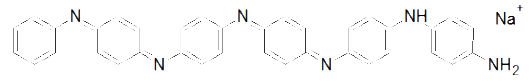
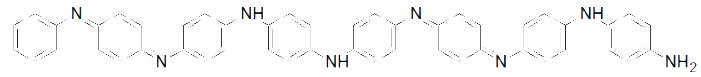
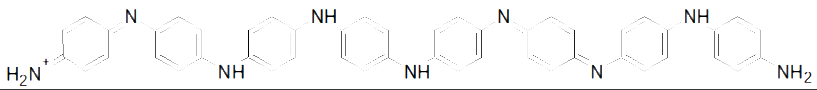
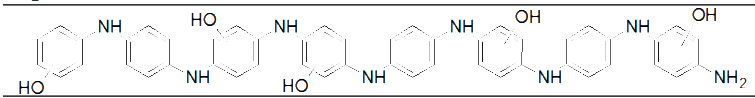
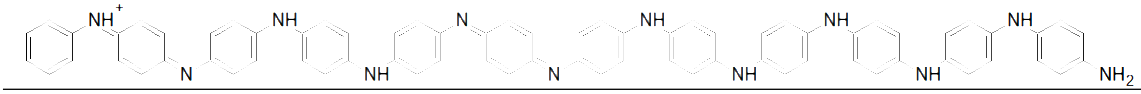


Figure S4. UV-vis spectra of all composites acquired **A**) in DMF solution and **B**) in DMF acidified with HCl; UV-vis spectra of PANI_ref compared to 1 × 1 sample **C**) in DMF and **D**) in DMF with HCl.

Table S2. Dependence of the H1/H2 ratio from the H_2O_2/aniline dimer molar ratio.

Sample	H_2O_2/Dimer	H1/H2
1x1	1	1.96
2x1	1	2.23
3x1	1	1.97
2x2	2	2.26
1x2	2	2.34
3x3	3	2.92
1x3	3	2.69

Table S3. Proposed structures attributed to main ESI-MS peaks.

	m/z
	366
	378
	406
	434
	567
	727
	743
	811
	1092

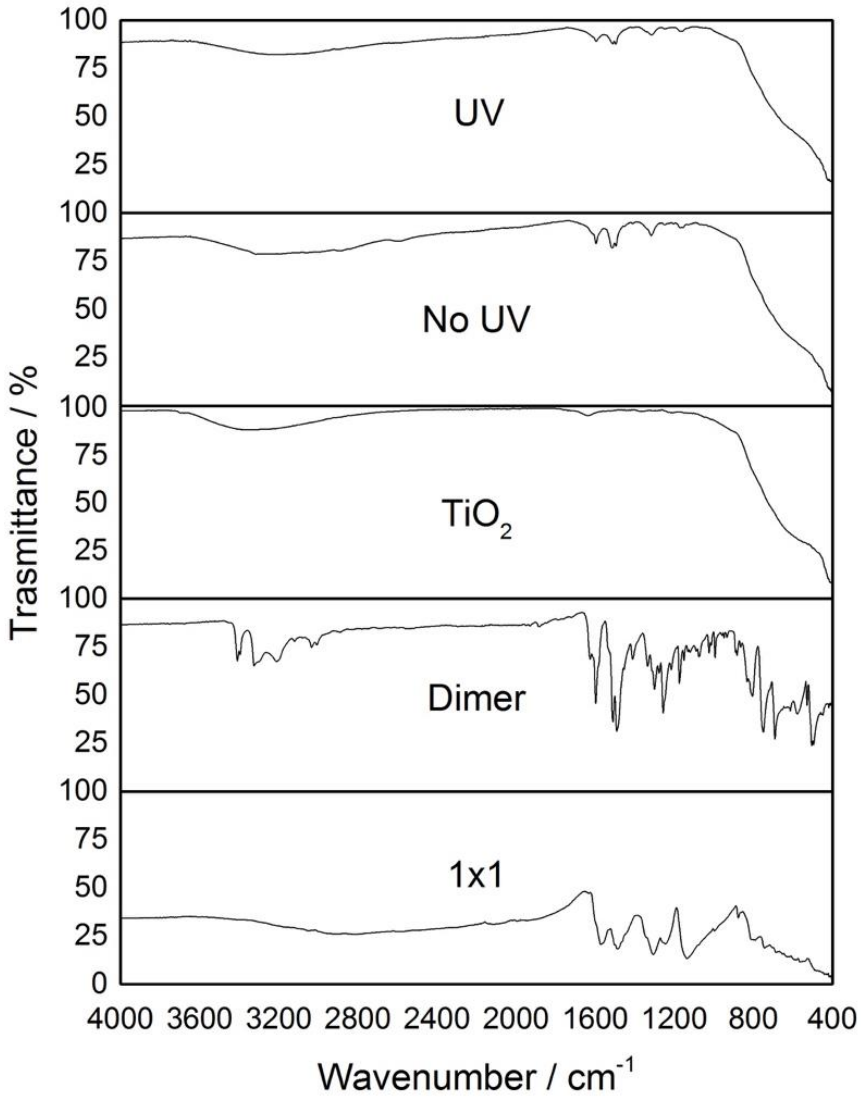


Figure S5. FT-IR spectra of the two tests studying the oligomerization step: tests under UV irradiation (UV) and in the dark (NoUV). The spectra of the pristineTiO_2, the aniline dimer and the 1 × 1 composite are reported for the sake of comparison.

Table S4. Surface elemental composition, determined from the XPS survey spectra, of NoUV, UV and pristine TiO_2 samples.

	C/Ti	**O/Ti**	**N/Ti**
No UV	2.6	2.6	0.19
UV	2.0	2.6	0.16
TiO_2	1.6	2.7	-

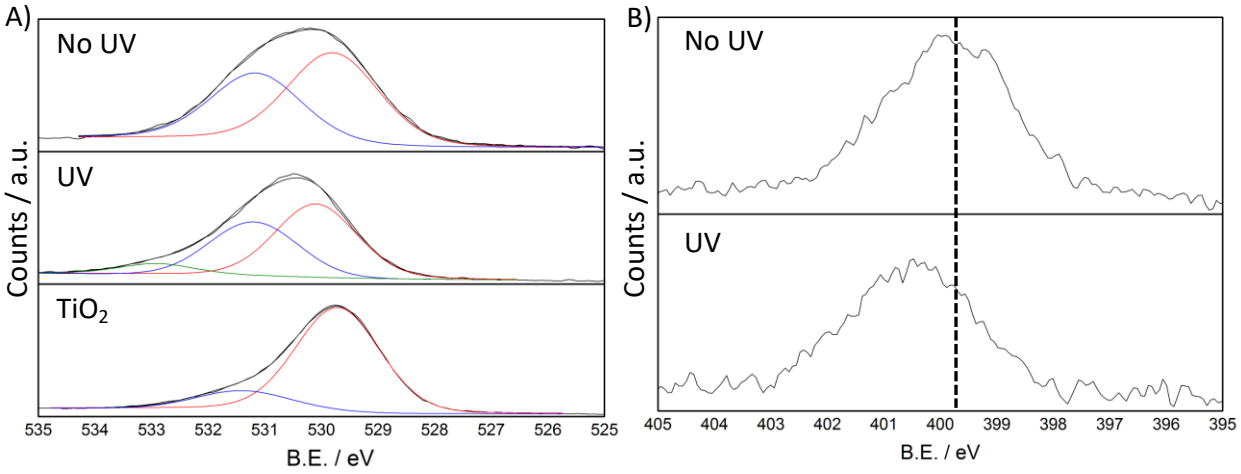


Figure S6. XPS spectra of the UV, NoUV and pristine TiO_2 samples in the **A**) O 1s and **B**) N 1s regions; the vertical line is added only as a guide for the eyes.

Table S5. Percentage of MO removed (± 2%) during sorption tests (50 mg composite, 20 mL of 50 ppm MO solution, 20 min).

Sample	$MO_{removed}$ /%
1 × 1	96
2 × 2	97
3 × 3	85
2 × 1	96
3 × 1	96
1 × 2	92
1 × 3	48

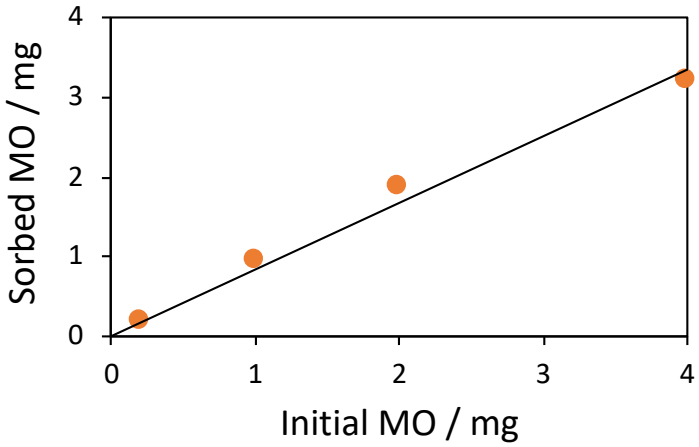


Figure S7. Sorbed MO amount as a function of the MO content of the initial solution for 1 × 1 sample.