Supplementary Information for:

Photocatalytic and surface properties of titanium dioxide nanoparticles in soil solutions

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2. Materials and methods

Soil analysis

The pH was measured after mixing deionized water with the soil sample in a mass ratio of 1:2.5 using a digital pH meter (Inolab pH 720)[1]. The determination of the soil texture is based on the plasticity index values according to Arany (Arany plasticity index). The index value is calculated from the amount (cm^3) of deionized water added to an air-dry soil sample (100 g) until reaching the upper limit of its plasticity, which is the moisture content at which a fine-grained soil can no longer be remolded without cracking[2,3,4]. The electrical conductivity (E_c) and the total salt content were analyzed using an Orion 3-Star (Thermo Electron Corporation) conductivity meter. The soil samples were saturated in water (± 10 $\mu S \cdot cm^{-1}$).

The organic matter (OM) contents were determined using a UV–vis spectrophotometer (Spectronic Helios-γ, Thermo Fisher Scientific) after oxidation of the organic matter with 0.33 M $K_2Cr_2O_7$ in the presence of 95% H_2SO_4 overnight. As a result, the organic carbon content of the soil sample was oxidized, while Cr^{6+} ions were reduced to Cr^{3+} ions. The concentration of Cr^{3+} ions was measured at a wavelength of 590 nm, which is directly proportional to the organic carbon content[5].

To determine the concentration of different major and trace elements (Na, K, Ca, Mg, Al, Fe, Mn, Zn, Cu, Ni, Co and As), 0.5 g of samples were weighted into a perfluoroalkoxy (PFA) vessel, and 7 mL aqua regia (HNO_3/HCl = 1:3) was added. The soil samples were digested in a microwave oven (Anton Paar Multiwave 3000). The concentrations of the elements were determined by an ICP-OES (Optima 7000 DV, PerkinElmer) (± 10% uncertainty)[6].

Table S1

GPS coordinates of soil samples

Sample name (in the figure)	GPS coordinates
Cs1 (1)	46°29'57.2"N, 20°12'28.3"E
Cs2 (2)	46°29'58.0"N, 20°12'32.6"E
Cs3 (3)	46°29'58.0"N, 20°12'30.1"E
Cs4 (4)	46°29'58.2"N, 20°12'30.0"E
Cs5 (5)	46°29'58.0"N, 20°12'28.0"E
Cs6 (6)	46°30'30.1"N, 20°12'32.0"E
Cs7 (7)	46°29'59.3"N, 20°12'31.3"E
Cs8 (8)	46°29'59.0"N, 20°12'29.0"E
Cs9 (9)	46°29'59.0"N, 20°12'27.1"E
Cs10 (10)	46°29'59.1"N, 20°12'26.0"E

Fig. S1. Location of the soil samples

3. Results and discussion

Table S2

Basic properties of the soil samples

Sample	pH d.w.*	Texture	Ec ($\mu S \cdot cm^{-1}$)	OM(%)*
Cs1	7.86	Sandy Loam	538	1.94
Cs2	7.82	Sandy Loam	471	2.42
Cs3	7.82	Sandy Loam	665	3.16
Cs4	7.81	Sandy Loam	670	3.1
Cs5	7.84	Sandy Loam	591	2.84
Cs6	7.9	Sandy Loam	482	3.22
Cs7	7.78	Loam	621	2.42
Cs8	7.81	Sandy Loam	542	2.72
Cs9	7.77	Loam	717	2.58
Cs10	7.74	Sandy Loam	715	2.7

Table S3

Total metal concentration of the soil samples

	mg·kg^{-1}											
Sample	**Cu**	**Zn**	**Co**	**Ni**	**Mn**	**Na**	**K**	**Ca**	**Mg**	**Al**	**Fe**	**As**
Cs1	24.48	72.84	8.02	26.80	577.96	359.1	12,45	26,59	10,13	32,46	25,45	11.44
Cs2	23.30	63.92	7.56	28.26	554.96	321.4	9,16	23,14	9,65	30,23	25,05	9.79
Cs3	22.90	55.61	7.57	24.78	554.76	399.5	10,42	24,65	9,87	34,8	26,44	9.81
Cs4	22.91	57.12	7.66	25.03	545.93	356.5	9,27	24	9,97	31,64	25,14	9.62
Cs5	22.68	55.16	7.47	24.58	544.98	303.6	8,64	24,36	9,55	29,83	24,58	9.62
Cs6	22.95	54.81	7.56	24.59	550.40	393.4	9,47	23,89	9,27	31,44	24,39	9.56
Cs7	23.03	54.82	7.55	24.39	550.02	320.1	11,35	22,9	9,25	29,89	24,39	9.66
Cs8	23.25	56.15	7.75	25.43	560.89	311.7	9,93	22,88	9,53	31,45	25,87	10.04
Cs9	26.54	58.69	7.77	25.13	554.88	382.6	9,87	24,69	10	33,22	25,85	9.67
Cs10	22.84	54.37	7.76	25.16	564.06	325.6	9,3	23,02	9,66	32,74	26,41	10.12

Table S4

Major and trace elements concentration of the soil solution samples

	μg·L^{-1}							
Sample	**Fe**	**Al**	**Mn**	**Zn**	**Co**	**Ni**	**Cu**	**As**
Cs1	38.58	63.67	4.87	11.15	0.34	6.86	11.58	13.76
Cs2	9.68	5.34	1.8	4.84	0.54	6.87	14.04	14.19
Cs3	5.55	1.59	1.11	5.46	0.36	5.83	12.51	11.18
Cs4	6.74	2.06	3.77	2.30	0.91	9.75	16.6	13.48
Cs5	5.99	0.03	0.72	2.78	0.27	6.08	13.5	13.64
Cs6	19.45	14.96	1.28	3.64	0.38	5.98	13.97	12.37
Cs7	37.64	39.91	3.71	5.23	0.6	5.5	14.4	12.13
Cs8	10.54	4.04	1.3	2.94	0.29	5.93	13.47	14.9
Cs9	8.09	1.77	0.61	2.81	0.37	5.63	11.05	11.93
Cs10	9.44	4.99	0.67	2.45	0.21	5.18	11.48	10.84

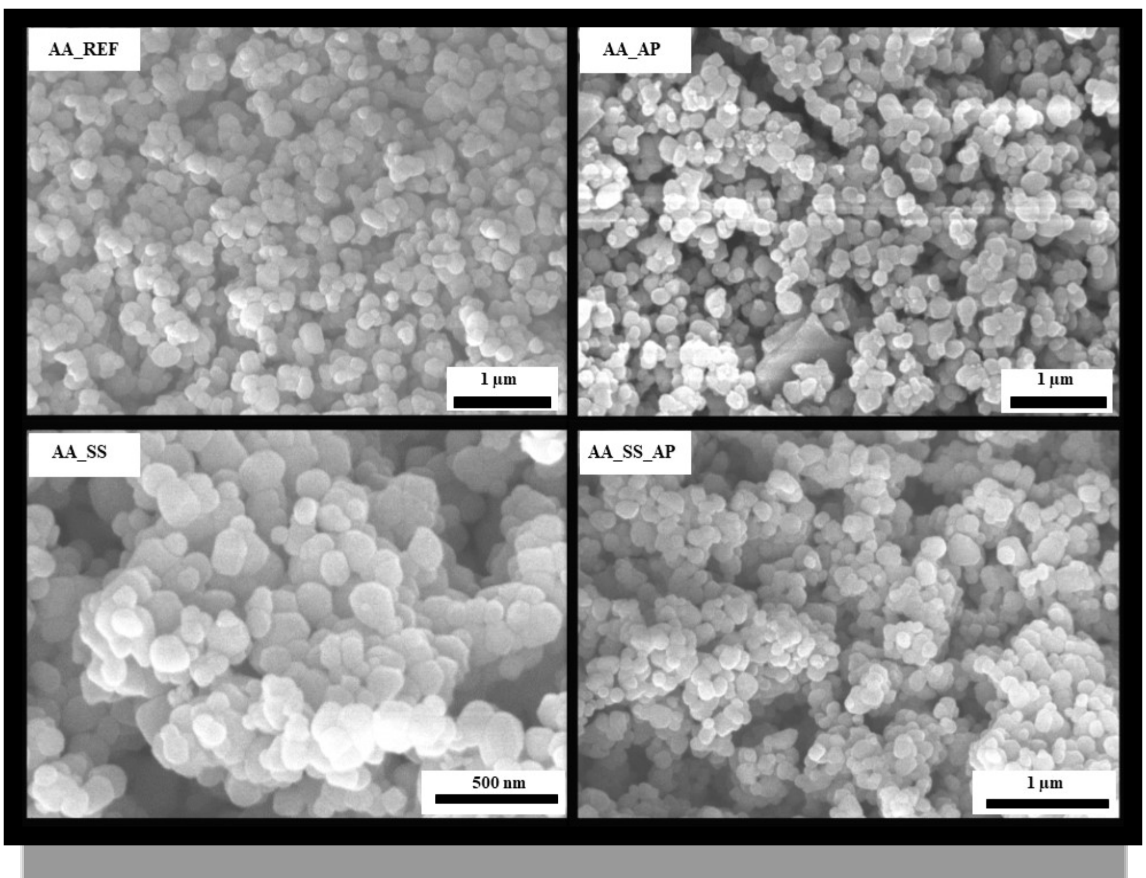

Fig. S2. SEM-micrographs of AA samples

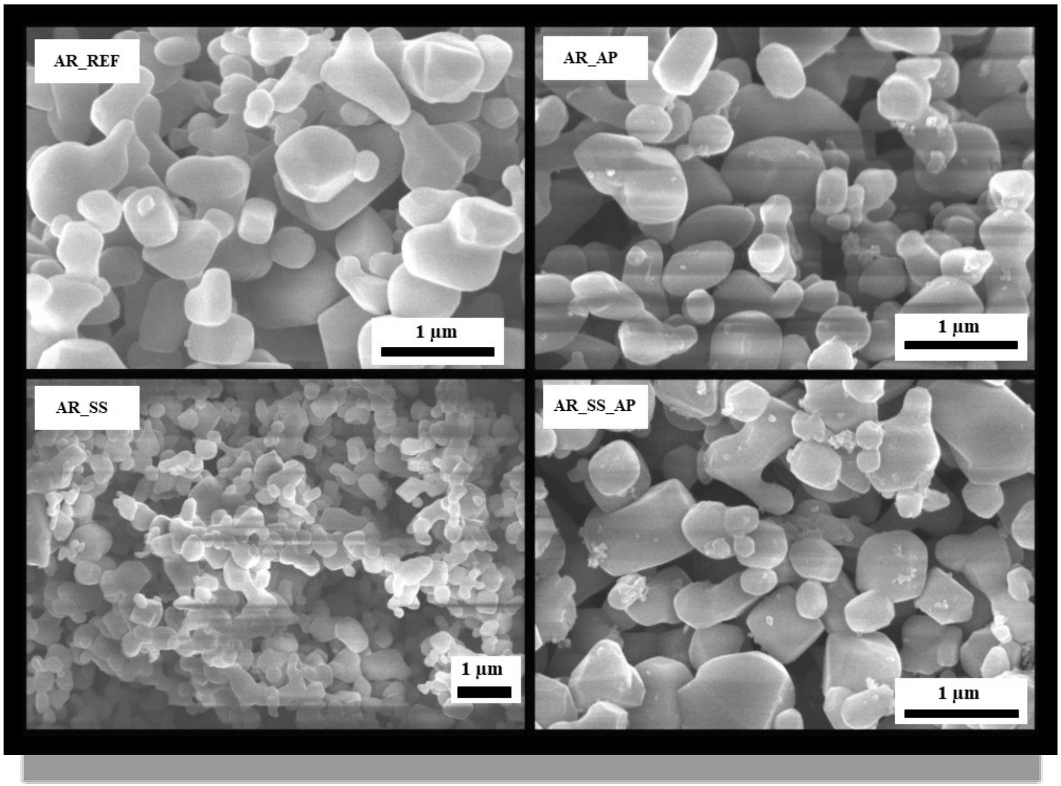

Fig. S3 SEM-micrographs of AA samples

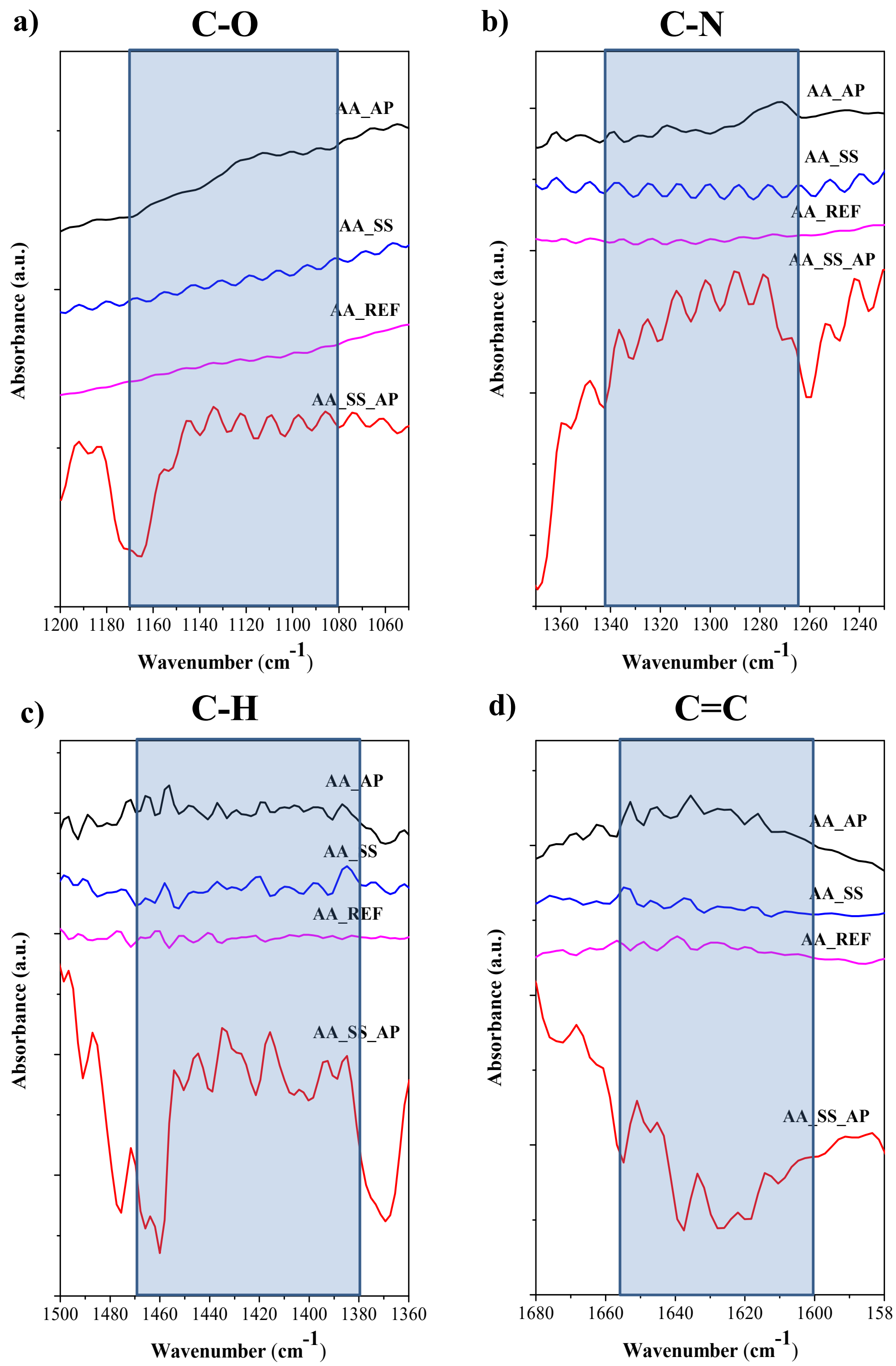

Fig. S4. IR spectras of AA samples: a) in the 1050-1200 cm^{-1} region; b) in the 1220-1380 cm^{-1} region; c) in the 1360-1500 cm^{-1} region; d) in the 1580-1680 cm^{-1} region

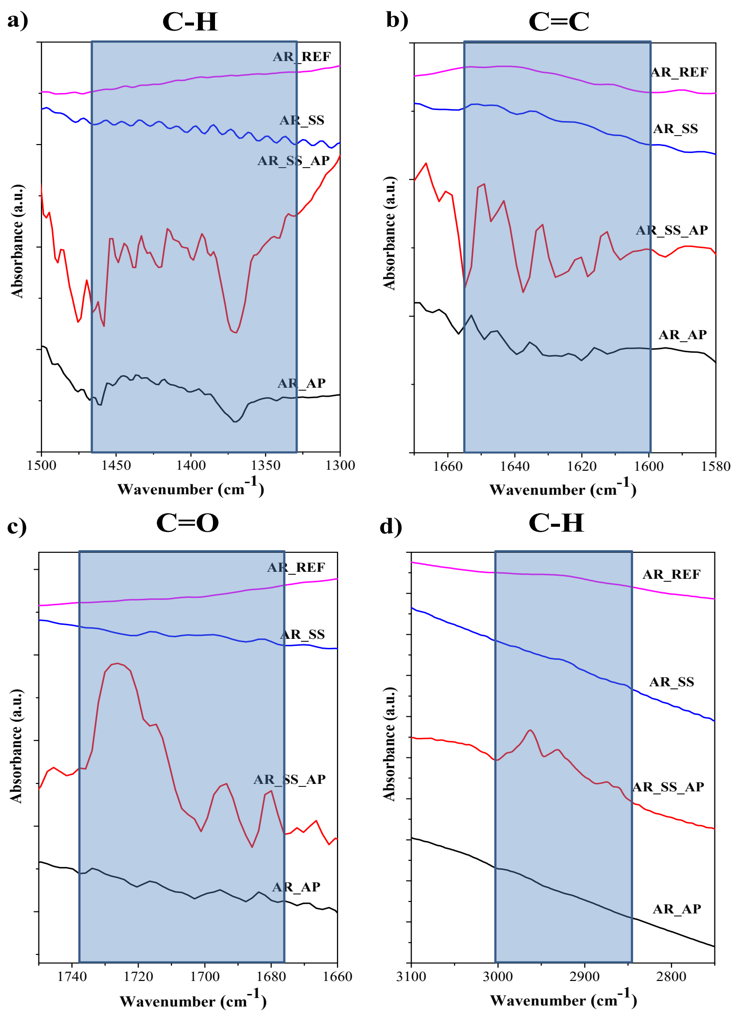

Fig. S5. IR spectras of AR samples: a) in the 1300-1500 cm^{-1} region; b) in the 1580-1660 cm^{-1} region; c) in the 1660-1750 cm^{-1} region; d) in the 2750-3100 cm^{-1} region

References

1. MSZ-08–0206–2, *Journal*, 1978.
2. MSZ-08–0205, *Journal*, 1978.
3. Z. Szolnoki, A. Farsang and I. Puskás, *Environmental Pollution*, 2013, **177**, 106-115.
4. N. T. H. Pham, I. Babcsányi and A. Farsang, *Environmental Geochemistry and Health*, 2022, **44**, 1893-1909.
5. MSZ-21470–52, *Journal*, 1983.
6. MSZ-21470-50, *Journal*, 2006.