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Ce ions surface-modified TiO_2 aerogel powders: a comprehensive study of their excellent photocatalytic efficiency in organic pollutants removal

Guru Karthikeyan Thirunavukkarasu,[a] Olivier Monfort,[a,*] Martin Motola,[a] Monika Motlochová,[b] Maroš Gregor,[c] Tomáš Roch,[c] Maria Čaplovicová,[d] Aleksandra Y. Lavrikova,[e] Karol Hensel,[e] Vlasta Brezová,[f] Monika Jerigová,[g,h] Ján Šubrt,[b] Gustáv Plesch[a]

Electronic Supplementary Information

[a.] *Department of Inorganic Chemistry, Faculty of Natural Sciences, Comenius University in Bratislava, Ilkovicova 6, Mlynska Dolina, 842 15 Bratislava, Slovakia*
[b.] *Institute of Inorganic Chemistry, Czech Academy of Sciences, Husinec-Rez c.p. 1001, 250 68 Rez, Czechia*
[c.] *Department of Experiment Physics, Faculty of Mathematics, Physics and Informatics, Comenius University in Bratislava, Mlynska Dolina, 842 48 Bratislava, Slovakia*
[d.] *STU Center for Nanodiagnostics, Slovak University of Technology in Bratislava, Vazovova 5, 812 43 Bratislava, Slovakia*
[e.] *Division of Environmental Physics, Faculty of Mathematics, Physics and Informatics, Comenius University in Bratislava, Mlynska Dolina, 84248, Bratislava, Slovakia*
[f.] *Institute of Physical Chemistry and Chemical Physics, Faculty of Chemistry and Food technology, Slovak University of Technology in Bratislava, Radlinskeho 9, 812 37 Bratislava, Slovakia*
[g.] *International Laser Centre, Ilkovicova 3, 842 48 Bratislava, Slovakia*
[h.] *Department of Physical and Theoretical Chemistry, Faculty of Natural Sciences, Comenius University in Bratislava, Ilkovicova 6, Mlynska dolina, 842 15 Bratislava, Slovakia*
** Corresponding author: monfort1@uniba.sk (email), +421(0)290142141 (phone)*

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Calculation of percentage of anatase phase present in P25 sample:

The P25 samples consist of ~82% of anatase phase, which is calculated using the formula [1]:

$$W_A = \frac{1}{1 + 1.26\,(\frac{I_R}{I_A})}$$

where, I_R and I_A is the strongest intensity of the rutile (110) and anatase (101) diffraction peak, respectively.

Table S1: Summary of Ce modified TiO_2 for photocatalytic application.

Material	Synthesis Technique	Ce Dopant Concentration	Bandgap (eV)	Type of Pollutant	Degradation %	Ref.
Ce^{3+}–TiO_2 catalysts	Sol-gel	0.7% atomic ratio (Ce/Ti)	Not calculated. But adsorption increased in the 400-500 nm region	• 2-mercaptobenzothiazole • Visible Light • 1.1 h	100	[2]
Ce-TiO_2	Sol-gel	0.4wt% (Ce/TiO_2)	Not calculated. But adsorption increased in the 400-500 nm region	• Phenol • UV light • 3 h	100	[3]
Ce^{3+} doped TiO_2	Precipitation	1.47wt% (EDX)	3.15	• Orange II dye • 400 nm • 0.5 h	~40	[4]
Mesoporous Ce/TiO_2	Sol-gel	5 mol%	Not calculated. But adsorption increased in the 400-500 nm region	• Methylene blue (MB) • Visible light • 1 h	100	[5]
Cerium-doped SiO_2/TiO_2 nanofibers	Sol-gel and electrospinning	0.2% molar ratio (Ce/Ti)	Not calculated. But adsorption increased in the 400-500 nm region	• Methylene blue (MB) • Simulated sunlight • 2 h	~80	[6]
Ce doped TiO_2 nanosheets	Hydrothermal	0.5% molar ratio	~3	• Rhodamine B • UV-Visible light • 1 h	~90	[7]
Ce- and S-co-doped TiO_2	Sol-gel	0.04 g ($Ce(NO_3)_3.6H_2O$	2.66	• Acid Orange 7 (AO-7) • Visible Light • 5 h	100	[8]
Ce/N co-doped TiO_2	Hydrothermal	0.05 g ($Ce(NO_3)_3.6H_2O$	1.8	• Acid Orange 7 (AO-7) • Visible Light • 5 h	100	[9]
Sn/Ce co-doped TiO_2	Sol-gel	2 mol%	3.02	• Methylene blue (MB) • Solar light • 2 h	~80	[10]
Ce–TiO_2 P25	Hydrothermal	0.29 mol% (Ce/TiO_2)	3.25	• Methylene blue (MB) • Visible light • 2.4 h	~96	[11]
Ti^{3+}-TiO_2/Ce^{3+}-CeO_2 nanosheet	Hydrothermal	1.56 at % (XPS)	2.7	• Methyl orange (MO) and methylene blue (MB) • Visible light • 3 h	~99	[12]
$In_{0.2}$-$Ce_{0.2}/TiO_2$ aerogels	Sol-gel	0.45 at%	2.84	• Rhodamine B • Visible • 1.5 h	~96	[13]
Ce doped TiO_2	Sol-gel	0.5wt%	3.06	• Caffeine • Visible light • 2 h	~30	[14]
Ce–TiO_2 P25	Hydrothermal	0.5wt% (Ce/Ti)	2.4	• Methylene blue (MB) • Visible light • 1.3 h	~90	[15]
Ce-doped anatase TiO_2	Sol-gel	0.1 mol%	3.31	• Methylene blue (MB) • UV light • 24 h min	~90	[16]

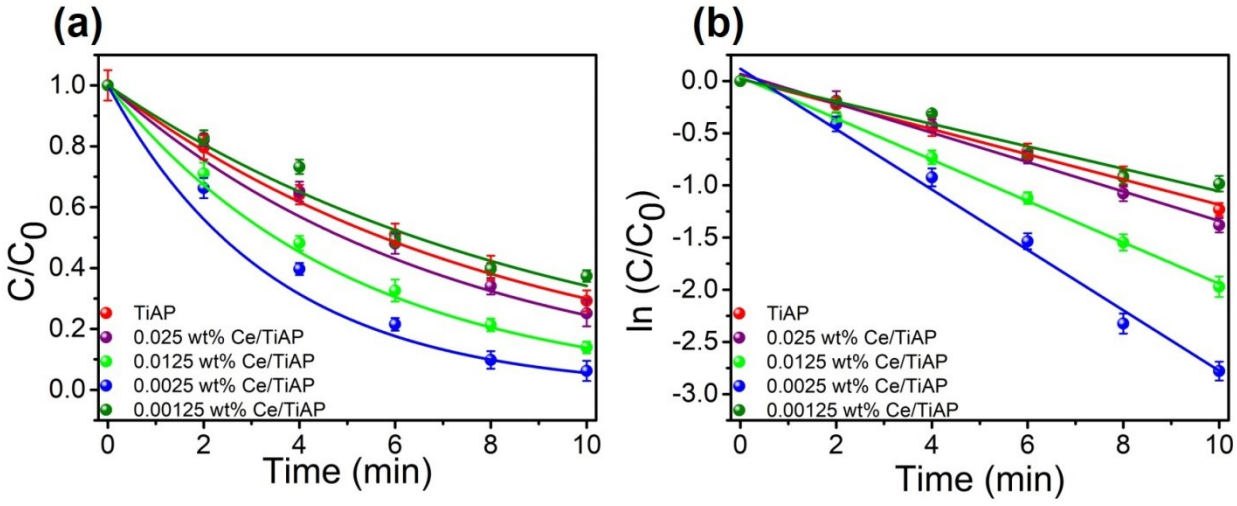

Figure S1: Influence of cerium ions surface-modification content on TiAP upon the photocatalytic efficiency in Rhodamine B decolorization under UVA light.

Table S2: The tabulation of photocatalytic activity rate (*k*) and degradation % of Rhodamine B under UVA light with different concentration of cerium surface modification on TiAP.

Sample	Photocatalytic activity rate (*k*) min^{-1}	Degradation %
TiAP	0.121	~71
0.025 wt% Ce/TiAP	0.141	~75
0.0125 wt% Ce/TiAP	0.198	~86
0.0025 wt% Ce/TiAP	0.289	~94
0.00125 wt% Ce/TiAP	0.107	~63

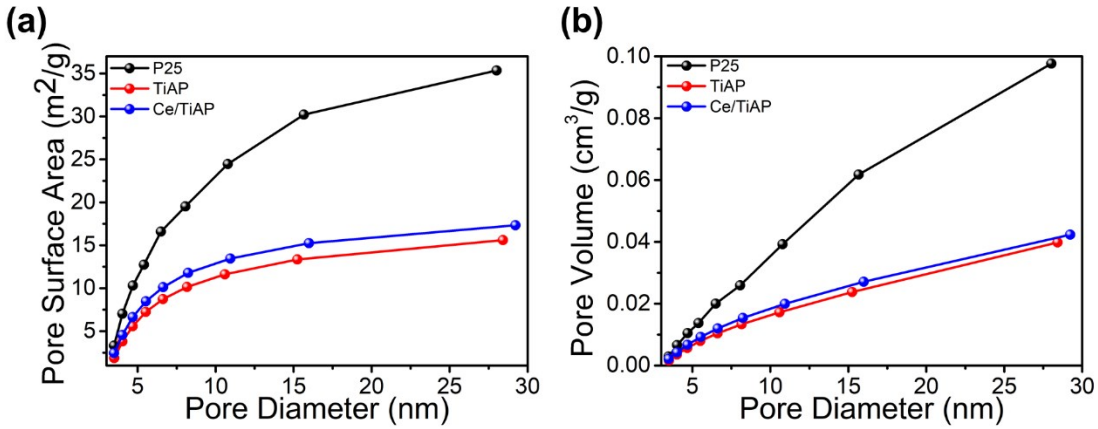

Figure S2: BET measurements of (a) Pore surface area and (b) pore volume respectively.

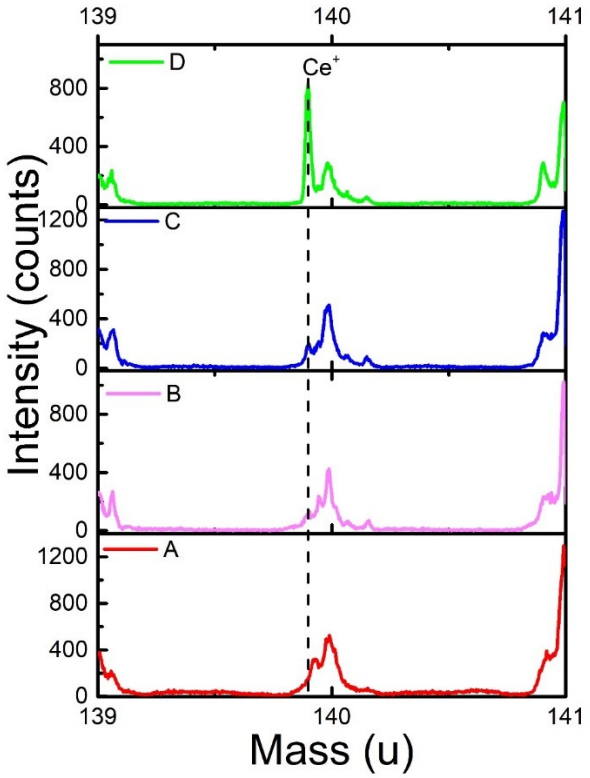

Figure S3: SIMS based detection of Ce in Ce/TiAP (A: Pristine TiAP, B: 0.00125 wt% Ce/TiAP, C: 0.0025 wt% Ce/TiAP and D: 0.0125 wt% Ce/TiAP). Ce^{+} ion peak was identified at 139.9 mu (dash line).

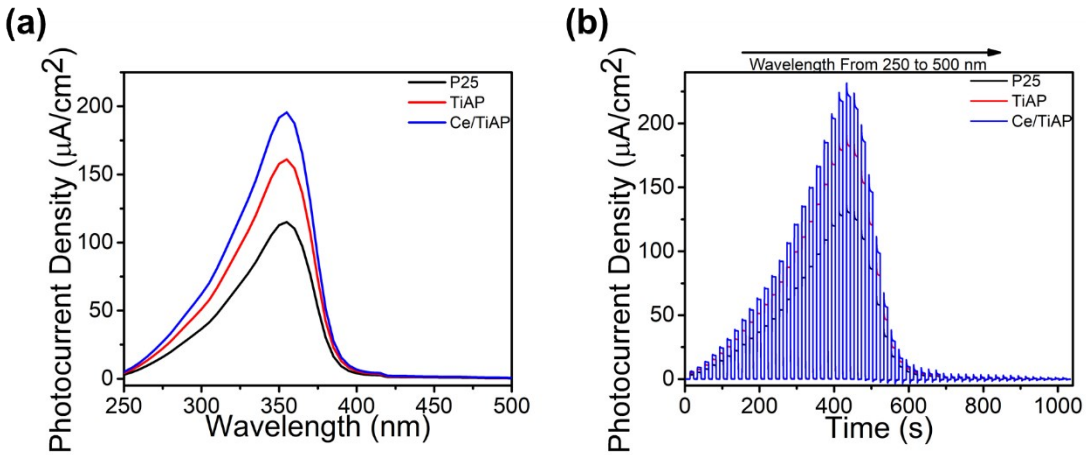

Figure S4: (a) Photocurrent densities of P25, TiAP and Ce/TiAP with (b) the corresponding transient current measured at 0.4 $V_{Ag/AgCl}$ in an aqueous 0.1 M Na_2SO_4 solution in the spectral range from 300 nm to 500 nm.

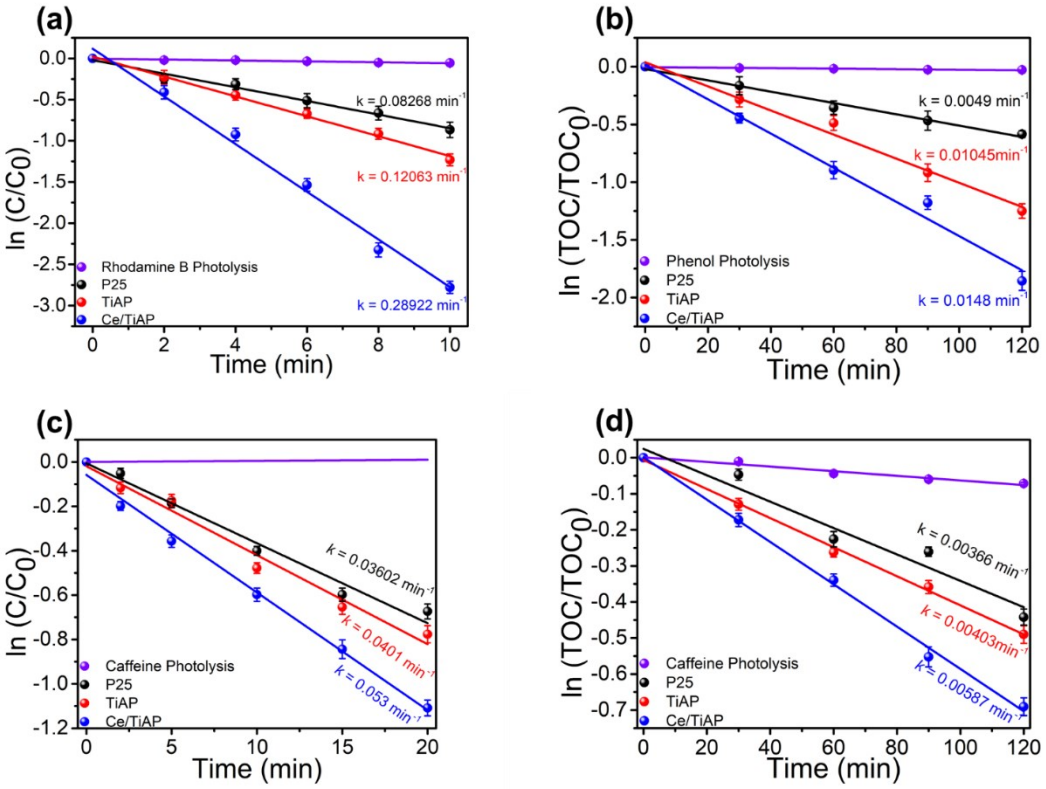

Figure S5: The linearized pseudo-first-order plots of $\ln(C/C_0)$ versus time (a) Rhodamine B, (b) Phenol mineralization measured by total organic carbon content analyzer, (c) & (d) Caffeine degradation by HPLC and mineralization measured by total organic carbon content analyzer.

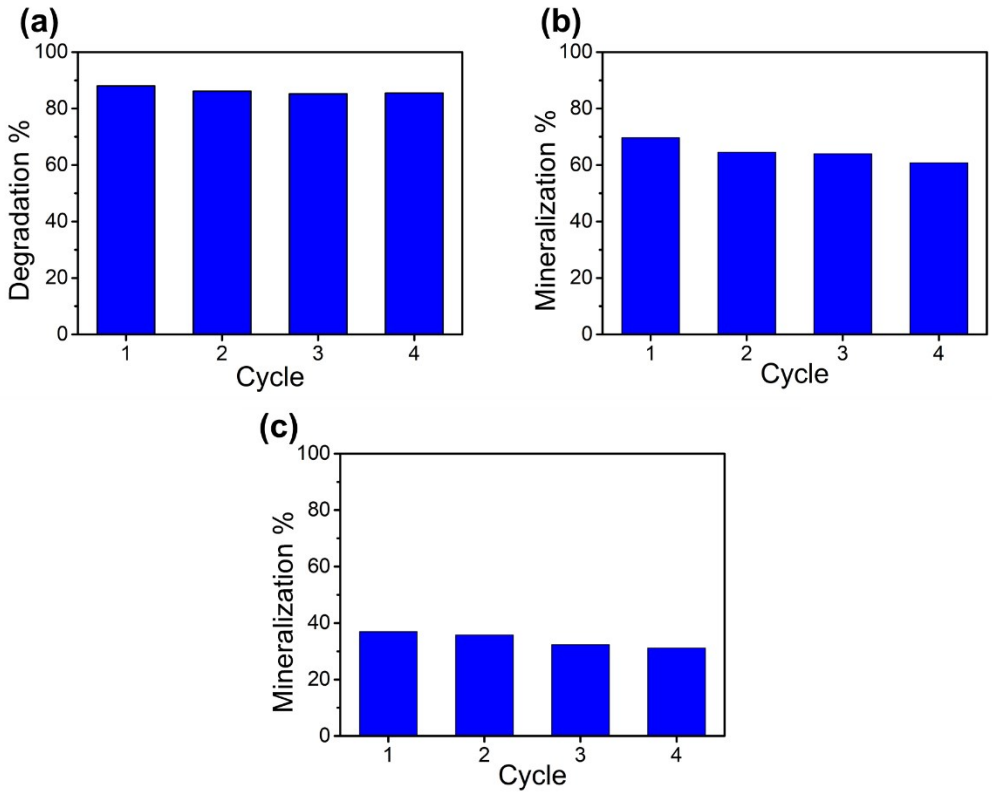

Figure S6: Repeated runs (4 cycles) using Ce/TiAP under UVA irradiation for the photocatalytic degradation of (a) Rhodamine B (C/C_0), (b) Phenol (TOC), (c) Caffeine (TOC).

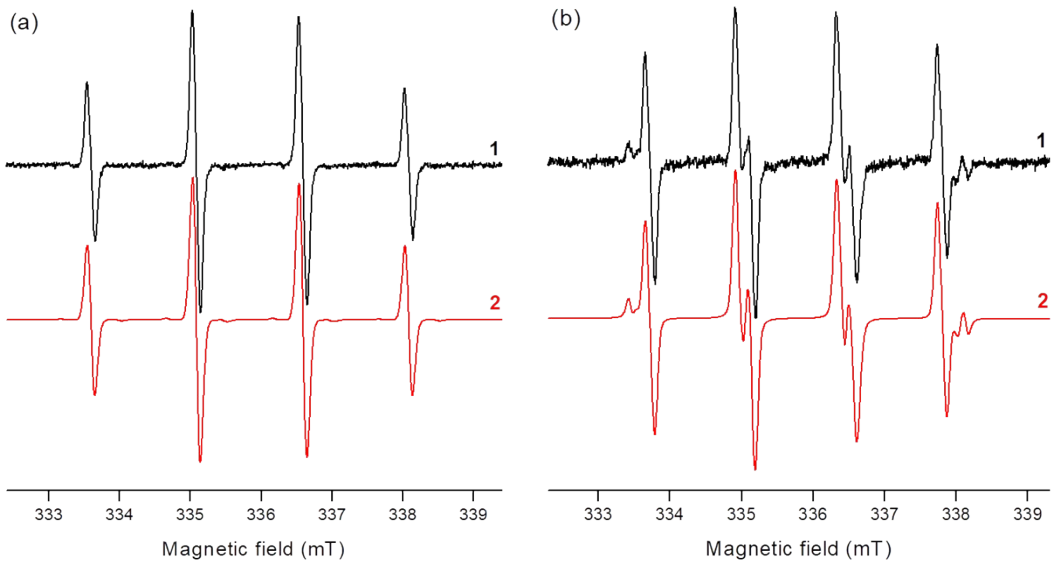

Figure S7: The normalized experimental (1) and simulated (2) EPR spectra obtained after 180 s exposure of aerated aqueous suspensions of TiAP in the presence of spin trapping agent: (a) DMPO; (b) BMPO. (LED@365 nm, irradiance 10 mW cm^{-2}; TiO_2 loading 0.2 mg mL^{-1}; c_0(DMPO) = 0.04 M; c_0(BMPO) = 0.02 M).

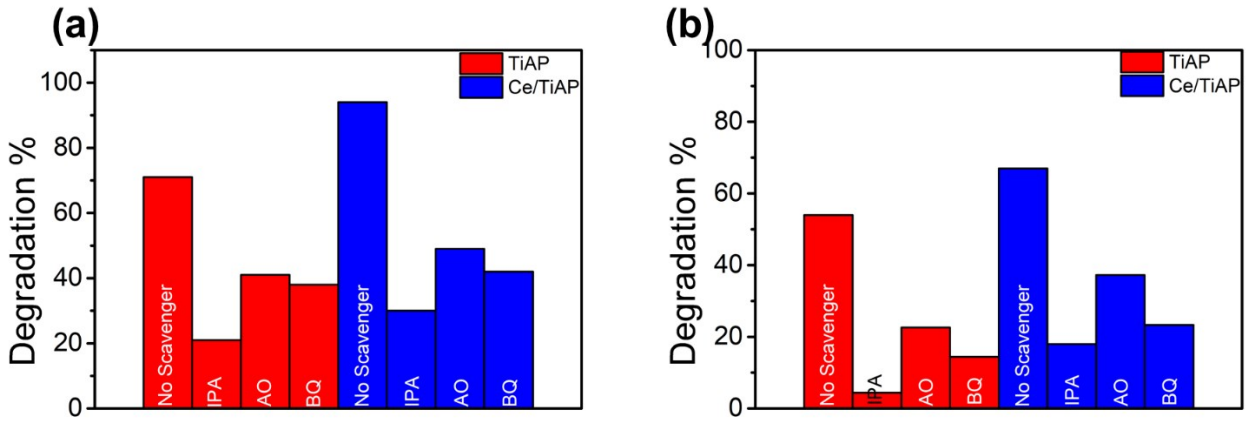

Figure S8: Free radical quenching of TiAP and Ce/TiAP using the isopropyl alcohol (IPA), ammonium oxalate (AO), benzoquinone (BQ) as scavengers (a) Rhodamine B and (b) caffeine.

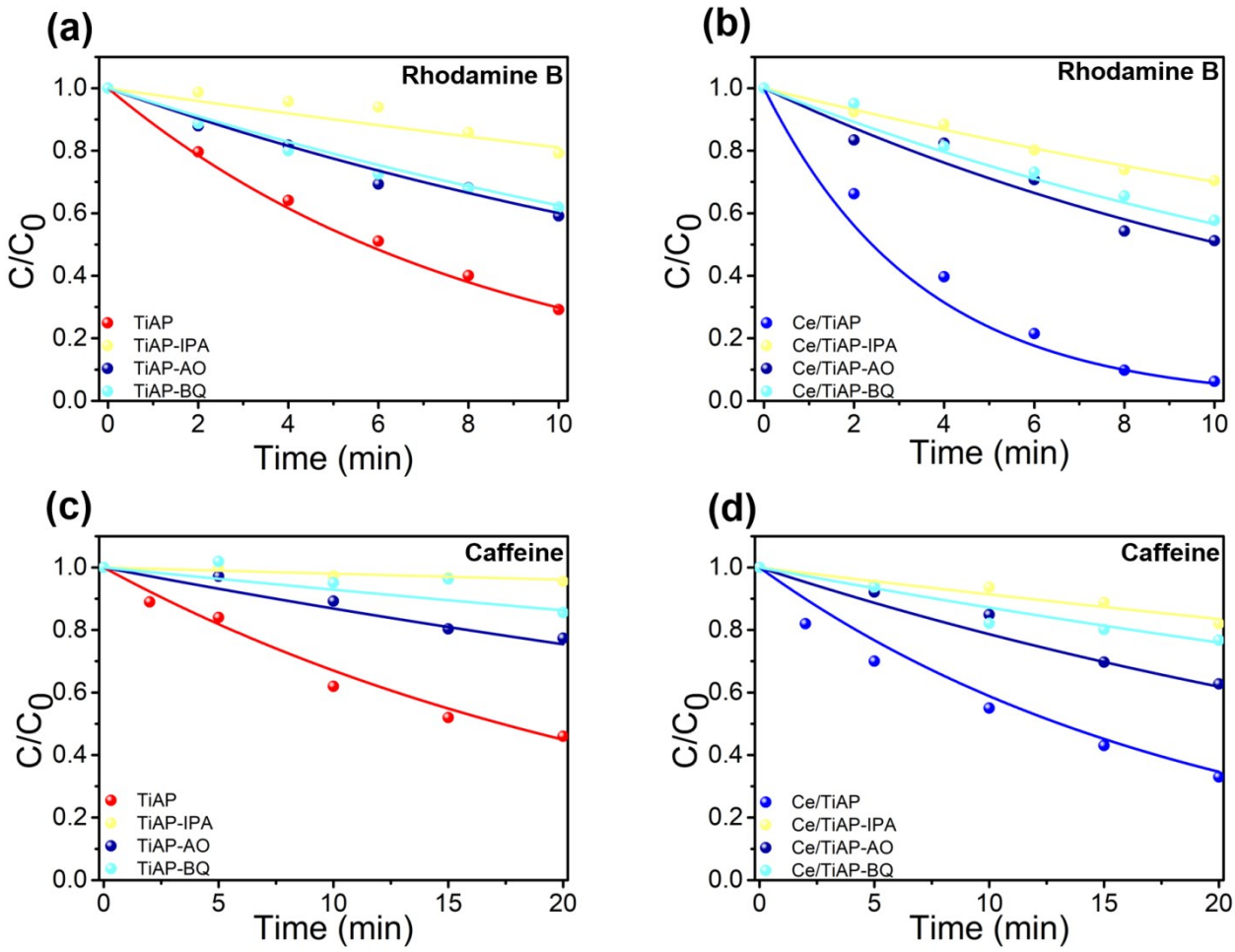

Figure S9: Degradation curves of (a) and (b) Rhodamine B and (c) and (d) Caffeine using TiAP and Ce/TiAP, respectively, under UVA irradiation.

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