

Supplementary Materials: The Role of Adsorption in the Photocatalytic Decomposition of Dyes on APTES-Modified TiO₂ Nanomaterials

Ewelina Kusiak-Nejman*, Agnieszka Sienkiewicz, Agnieszka Wanag, Paulina Rokicka-Konieczna and Antoni W. Morawski

Department of Inorganic Chemical Technology and Environment Engineering, Faculty of Chemical Technology and Engineering, West Pomeranian University of Technology in Szczecin, Pułaskiego 10, 70-322 Szczecin, Poland; Agnieszka.Sienkiewicz@zut.edu.pl (A.S.); awanag@zut.edu.pl (A.W.); prokicka@zut.edu.pl (P.R.-K.); amor@zut.edu.pl (A.W.M.)

* Correspondence: ekusiak@zut.edu.pl; Tel: +48 91 449 42 44

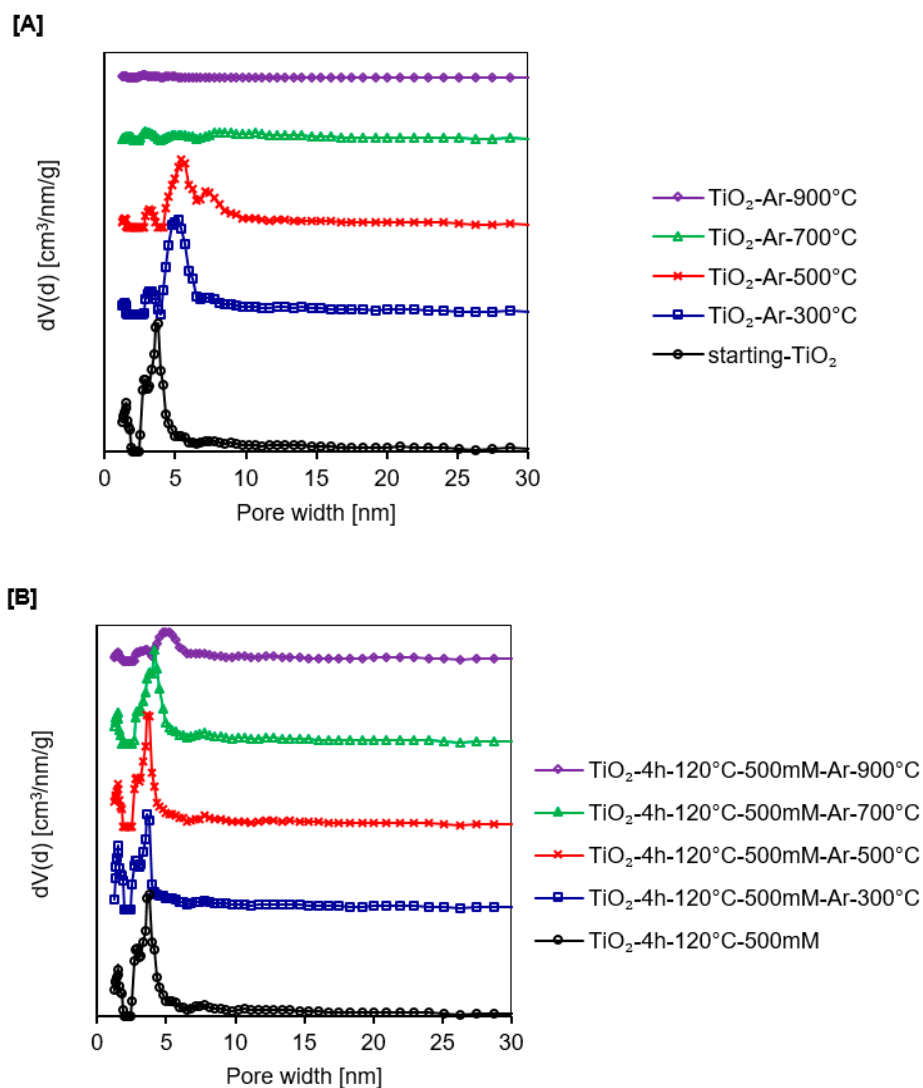


Figure S1. Pore size distribution plots of starting-TiO₂, calcined reference samples (A), and APTES-modified TiO₂ photocatalysts (B).

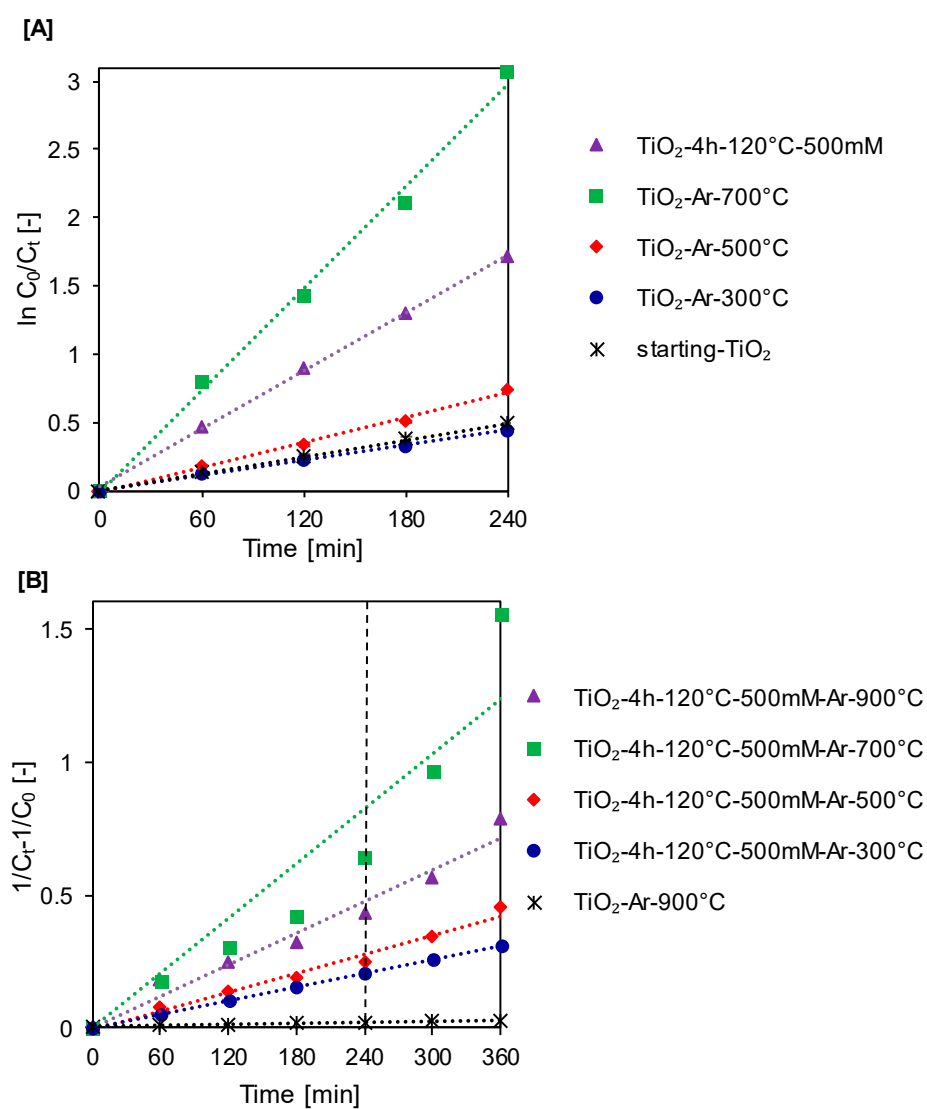


Figure S2. The pseudo-first-order plot (A), and the pseudo-second-order plot (B) of methylene blue decomposition.

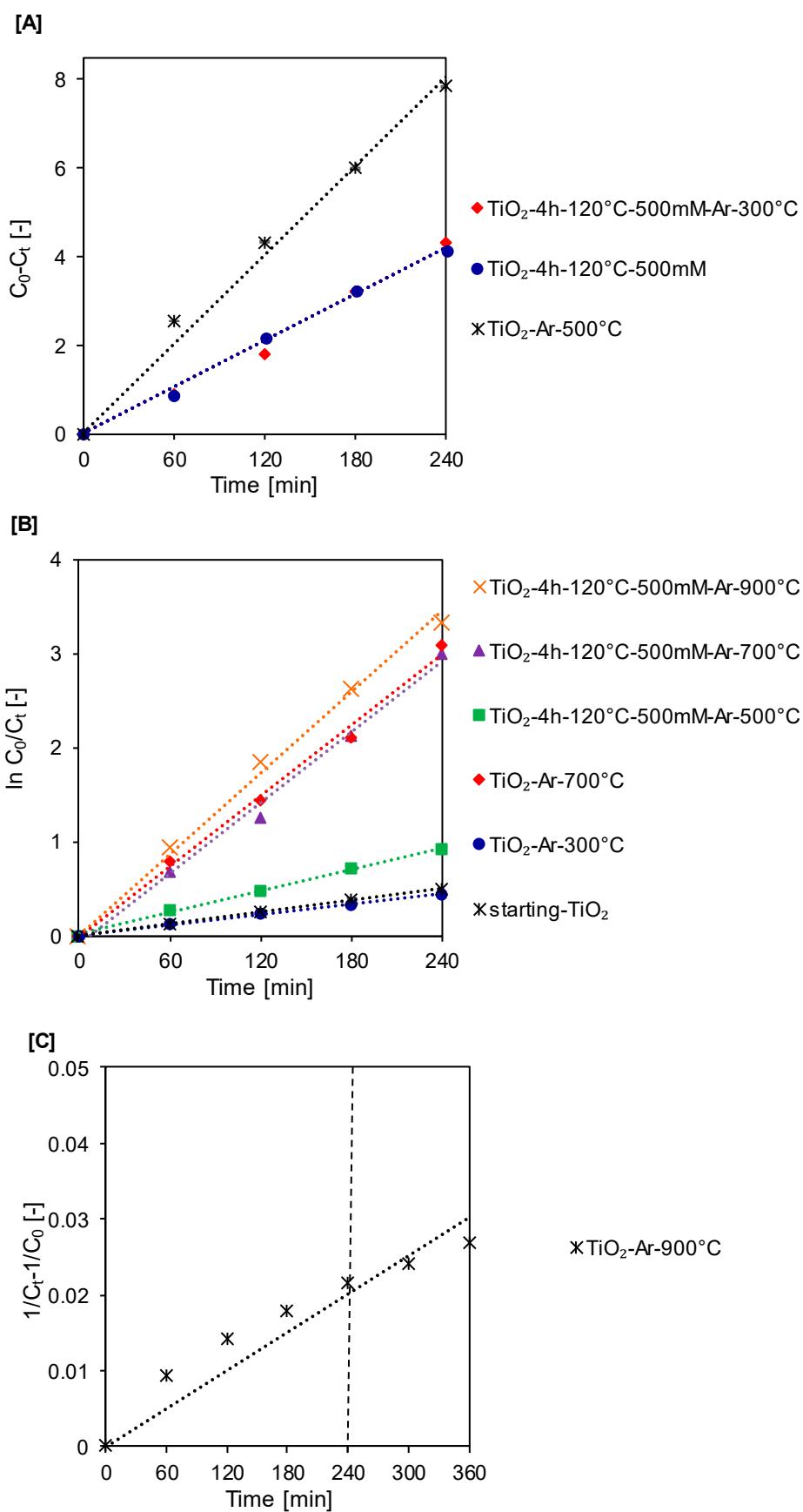


Figure S3. The zero-order plot (A), the pseudo-first-order plot (B), and the pseudo-second-order plot (C) of Orange II decomposition.

Table S1. Isotherm constants for the adsorption process of methylene blue on starting TiO₂, calcined reference samples and APTES-modified photocatalysts.

Sample name	Isotherm models												
	Freundlich			Langmuir			Langmuir-Freundlich			Temkin			
	K _F ((mg/g)·(L/mg) ^{1/n})	n	R ²	K _L (L/mg)	q _m (mg/g)	R ²	K _{LF} (L/mg)	q _m (mg/g)	n	R ²	K _T (L/mg)	B	R ²
starting TiO ₂	0.12	2.52	0.71	0.42	0.35	0.69	0.00	1.87	0.45	0.71	0.10	0.08	0.71
TiO ₂ -Ar-300°C	0.13	4.99	0.30	0.93	0.23	0.35	0.93	0.23	1.12	0.35	0.12	0.04	0.32
TiO ₂ -Ar-500°C	0.12	7.12	0.09	3.93	0.13	0.02	0.10	0.22	4.54	0.76	0.28	0.08	0.50
TiO ₂ -Ar-700°C	0.33	3.27	0.81	0.64	0.75	0.73	0.001	3.77	0.35	0.81	0.32	0.15	0.79
TiO ₂ -Ar-900°C	0.67	4.54	0.58	1.00	1.22	0.70	0.87	1.25	1.88	0.88	0.64	0.29	0.78
TiO ₂ -4h-120°C-500mM	0.29	16.44	0.24	4.33	0.34	0.29	1.48	0.37	2.28	0.24	0.28	0.01	0.73
TiO ₂ -4h-120°C-500mM-Ar-300°C	0.53	3.67	0.93	0.78	1.10	0.98	0.88	1.01	1.43	0.99	0.50	0.21	0.96
TiO ₂ -4h-120°C-500mM-Ar-500°C	2.98	3.64	0.91	1.50	5.21	0.99	1.49	5.22	1.00	0.99	3.05	0.93	0.91
TiO ₂ -4h-120°C-500mM-Ar-700°C	5.17	4.25	0.92	3.56	7.64	0.99	3.11	8.02	0.81	1.00	5.25	1.16	0.97
TiO ₂ -4h-120°C-500mM-Ar-900°C	6.43	7.04	0.82	19.29	7.92	0.93	24.19	7.61	0.78	0.91	6.70	0.89	0.89

Table S2. Isotherm constants for the adsorption process of Orange II on starting TiO₂, calcined reference samples and APTES-modified photocatalysts.

Sample name	Isotherm models												
	Freundlich			Langmuir			Langmuir-Freundlich			Temkin			
	K _F ((mg/g)·(L/mg) ^{1/n})	n	R ²	K _L (L/mg)	q _m (mg/g)	R ²	K _{LF} (L/mg)	q _m (mg/g)	n	R ²	K _T (L/mg)	B	R ²
starting-TiO ₂	0.003	0.31	1.00	0.0002	18.47	0.75	0.027	3.65	3.31	1.00	0.85	1.84	0.70
TiO ₂ -Ar-300°C	0.08	0.51	0.98	0.0004	18.69	0.95	0.004	19.49	1.97	0.98	0.68	1.86	0.77
TiO ₂ -Ar-500°C	0.02	0.39	1.00	0.0002	23.70	0.85	0.061	42.87	2.91	1.00	3.67	3.86	0.79
TiO ₂ -Ar-700°C	0.0006	0.01	0.95	0.0006	9.30	0.01	0.194	0.02	177	0.38	0.01	0.004	0.05
TiO ₂ -Ar-900°C	0.18	3.85	0.23	1.19	0.34	0.12	0.001	2.62	0.36	0.52	0.19	0.06	0.19
TiO ₂ -4h-120°C-500mM	0.25	0.66	0.98	0.0006	10.78	0.96	0.003	13.58	1.52	0.98	0.98	1.93	0.83
TiO ₂ -4h-120°C-500mM-Ar-300°C	1.07	2.38	0.98	0.04	11.85	0.95	0.001	51.13	0.58	0.94	1.16	0.67	0.94
TiO ₂ -4h-120°C-500mM-Ar-500°C	0.84	3.72	0.99	0.94	1.70	0.90	0.001	7.75	0.32	0.99	0.85	0.31	0.97
TiO ₂ -4h-120°C-500mM-Ar-700°C	0.67	7.79	0.82	3.32	0.90	0.57	0.001	2.86	0.18	0.81	0.67	0.10	0.79
TiO ₂ -4h-120°C-500mM-Ar-900°C	0.18	3.85	0.23	1.19	0.34	0.12	0.001	2.62	0.36	0.52	0.19	0.06	0.19

Table S3. The fitting parameters, the pseudo-first and pseudo-second reaction rate constants for methylene blue photoremoval (after 240 min of UV radiation).

Sample name	k_1 (L/min)	R^2	Sample name	k_2 (L/(min·mg))	R^2
TiO ₂ -Ar-300 °C	0.0019	0.99	TiO ₂ -Ar-900 °C	0.0001	0.92
starting TiO ₂	0.0021	0.99	TiO ₂ -4h-120 °C-500mM-Ar-300 °C	0.0009	0.99
TiO ₂ -Ar-500 °C	0.0030	0.99	TiO ₂ -4h-120 °C-500mM-Ar-500 °C	0.0011	0.99
TiO ₂ -4h-120 °C-500mM	0.0072	0.99	TiO ₂ -4h-120 °C-500mM-Ar-900 °C	0.0019	0.94
TiO ₂ -Ar-700 °C	0.0124	0.99	TiO ₂ -4h-120 °C-500mM-Ar-700 °C	0.0025	0.99

Table S4. The fitting parameters, zero, pseudo-first, and pseudo-second reaction rate constants for Orange II photoremoval (after 240 min of UV radiation).

Sample name	k_0 (mg/(L·min))	R^2	Sample name	k_1 (1/min)	R^2	Sample name	k_2 (L/(min·mg))	R^2
TiO ₂ -4h-120 °C-500mM	0.0171	0.99	TiO ₂ -Ar-300 °C	0.0019	0.99	TiO ₂ -Ar-900 °C	0.0001	0.92
TiO ₂ -4h-120 °C-500mM-Ar-300 °C	0.0175	0.99	starting-TiO ₂	0.0021	0.99			
TiO ₂ -Ar-500 °C	0.0337	0.99	TiO ₂ -4h-120 °C-500mM-Ar-500 °C	0.0039	0.99			
			TiO ₂ -4h-120 °C-500mM-Ar-700 °C	0.0114	0.99			
			TiO ₂ -Ar-700 °C	0.0124	0.99			
			TiO ₂ -4h-120 °C-500mM-Ar-900 °C	0.0143	0.99			

