



Supplementary Materials

Synthesis of N-Doped TiO₂ for Efficient Photocatalytic Degradation of Atmospheric NO_x

Tamal Tahsin Khan ^{1,2}, Gazi A. K. M. Rafiqul Bari ¹, Hui-Ju Kang ¹, Tae-Gyu Lee ¹, Jae-Woo Park ¹, Hyun Jin Hwang ³, Sayed Mukit Hossain ⁴, Jong Seok Mun ¹, Norihiro Suzuki ⁵, Akira Fujishima ⁵, Jong-Ho Kim ³, Ho Kyong Shon ^{4,*} and Young-Si Jun ^{1,3,*}

- ¹ Department of Advanced Chemicals & Engineering, Chonnam National University, 77 Yongbong-ro, Buk-gu, Gwangju 61186, Korea; tamalche15@gmai.com (T.T.K.); grafiqulbari@gmail.com (G.A.K.M.R.B.); gmlwn120@gmail.com (H.-J.K.); dlxorb007@gmail.com (T.-G.L.); jaewopark0218@gmail.com (J.-W.P.); answhdtjr8726@gmail.com (J.S.M.)
- ² Department of Materials Science and Engineering, Chonnam National University, 77 Yongbong-ro, Buk-gu, Gwangju 61186, Korea
- ³ School of Chemical Engineering, Chonnam National University, 77 Yongbong-ro, Buk-gu, Gwangju 61186, Korea; wgguswls@gmail.com (H.J.H.); jonghkim@jnu.ac.kr (J.-H.K.)
- ⁴ Faculty of Engineering and IT, University of Technology, Sydney, P.O. Box 123, Broadway, NSW 2007, Australia; sayed.m.hossain@student.uts.edu.au
- ⁵ Photocatalysis International Research Center (PIRC), Research Institute for Science and Technology (RIST), Tokyo University of Science, 2641 Yamazaki, Noda, Chiba 278-8510, Japan;
- suzuki.norihiro@rs.tus.ac.jp (N.S.); fujishima_akira@rs.tus.ac.jp (A.F.)
 * Correspondence: Hokyong.Shon-1@uts.edu.au (H.K.S.); ysjun@jnu.ac.kr (Y.-S.J.);
- Correspondence: Hokyong.Snon-1@uts.edu.au (H.K.S.); ysjun@jnu.ac.kr (Y.-Tel.: +61-2-95142629 (H.K.S.); +82-62-530-1812 (Y.-S.J.)

Citation: Khan, T.T.; Bari, R.; Kang, H.-J.; Lee, T.-G.; Park, J.-W.; Hwang, H.J.; Hossain, S.M.; Mun, J.S.; Suzuki, N.; Fujishima, A.; et al. Synthesis of N-doped TiO₂ for Efficient Photocatalytic Degradation of Atmospheric NO₆. *Catalysts* **2021**, *11*, 109. https://doi.org/10.3390/ catal1101009

Received: 15 December 2020 Accepted: 12 January 2021 Published: 14 January 2021

Publisher's Note: MDPI stays neutral with regard to jurisdictional claims in published maps and institutional affiliations.



Copyright: © 2021 by the authors. Submitted for possible open access publication under the terms and conditions of the Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by/4.0/).



Figure S1. The broad scan survey spectra of pure TiO₂ P25 and N-doped TiO₂ samples with 10 wt% and 50 wt% nitrogen contents.



Figure S2. N2 adsorption desorption isotherm of pure TiO2 P25 and synthesized N-doped TiO2.





Figure S3. Emission spectra of (a) UV, and (b) visible light sources.

Commiss	Position	FWHM	Crystal size	BET surface area	Pore volume
Samples	(20)	(20)	(nm)	(m²/g)	(cc/g)
TiO ₂ P25	25.36	0.4905	16.60	52.21	0.20
TC7.5	25.37	0.4723	17.24	58.50	0.52
TC10	25.35	0.4445	18.32	50.98	0.46
TC25	25.35	0.4433	18.37	47.69	0.43
TC50	25.38	0.4393	18.54	45.24	0.37

Table S1: Estimated FWHM and crystal size of the prepared samples along with the anatase (101) plane of TiO₂, and BET surface area and pore volume from N₂ adsorption desorption isotherm.

Table S2. XPS elemental analysis of purer TiO₂ P25 and N-doped TiO₂ samples with 10wt% and 50wt% nitrogen contents.

Sample	Ti2p (atomic %)	O1s (atomic %)	N1s (atomic %)	C1s (atomic %)
TiO ₂ P25	23.18	76.82	0	0
TC10	21.88	53.84	2.1	22.19
TC50	18.57	46.41	8.9	26.12

 Table S3: The energy band gap, CB and VB edge potential of pure TiO2 P25 and N-doped TiO2 samples. The CB and VB edge potentials was measured vs Ag/AgCl at pH 5.8 and calculated vs NHE at pH 7.

Sample	CB potential (V)		Energy band gap (eV)	VB potential (V)	
	Ag/AgCl pH 5.8	NHE pH 7		Ag/AgCl pH 5.8	NHE pH 7
TiO ₂ P25	-0.80	-0.66	3.25	2.45	2.59
TC7.5	-0.83	-0.66	3.22	2.39	2.56
TC10	-0.87	-0.66	3.18	2.31	2.52
TC25	-0.91	-0.66	3.14	2.23	2.48
TC50	-0.98	-0.66	3.10	2.12	2.44

-	Sample	NO removal (%)	NO ₂ generation (%)	NO _x removal (%)	N03- selectivity (%)
-	TiO ₂ P25	47	29	17	36
	TC7.5	49	17	32	65
	TC10	59	25	34	58
	TC25	51	23	29	57
	TC50	41	21	20	49

Table S4: Photocatalytic efficiency of samples in NO removal, NO₂ generation, NO_x removal and NO₃⁻ selectivity under UV irradiation.

Table S5: Photocatalytic efficiency of samples in NO removal, NO₂ generation, NO_x removal and NO₃⁻ selectivity under visible light irradiation.

Sample	NO removal (%)	NO ₂ generation (%)	NOx removal (%)	N03 ⁻ selectivity (%)
TiO2 P25	20	7	13	65
TC7.5	46	24	22	48
TC10	51	22	28	55
TC25	48	32	16	33
TC50	21	5	16	76