Electronic Supplementary Information (ESI) for

Synthesis of a UiO-66/g-C₃N₄ composite using terephthalic acid obtained from waste plastic for the photocatalytic degradation of chemical warfare agent simulant, methyl paraoxon

Dung Van Le^{a,b}, Manh B. Nguyen^{c*}, Phuong T. Dang^c, Taeyoon Lee^{d*}, Trinh Duy Nguyen^{a,d*}

^aGraduate University of Science and Technology, Academy of Science and Technology, 18 Hoang Quoc Viet Street, Cau Giay, Ha Noi, Vietnam.

^bCenter for Technology Environmental Treatment, 282 Lac Long Quan Street, Tay Ho, Ha Noi, Vietnam

^cInstitute of Chemistry, Vietnam Academy of Science and Technology, 18 Hoang Quoc Viet Street, Cau Giay, Ha Noi, Vietnam.

^dDepartment of Environmental Engineering, College of Environmental and Marine, Pukyong National University, 45 Yongso-ro, Nam-gu, Busan, 48513, Republic of Korea

^eInstitute of Applied Technology and Sustainable Development, Nguyen Tat Thanh University, Ho Chi Minh City, Vietnam

Corresponding author: nguyenbamanh@ich.vast.vn (Manh B. Nguyen), badger74w@pknu.ac.kr (Taeyoon Lee) and <u>ndtrinh@ntt.edu.vn</u> (Trinh Duy Nguyen).



Fig. S1. HPLC spectrum of H₂BDC product.



Fig. S2. Schematic synthesis of UiO-66/g- C_3N_4 materials by solvothermal method



Fig. S3. XRD pattern of g-C₃N₄ sample



Fig. S4. SEM images of g-C $_3N_4$, UiO-66 and UiO-66/g-C $_3N_4$ samples



Fig. S5. (A) EDS spectra of UiO-66 and (B) UiO-66/g- C_3N_4 -30 (B) samples



Fig. S6. Degradation of DMNP by UiO-66 and UiO-66/g-C₃N₄



Fig. S7. UV-Vis spectra the degradation of DMNP using UiO-66/g-C₃N₄-30% sample.



Fig. S8. Images of DMNP samples in 0.15M N-ethylmorpholine buffer at different times



Fig. S9. LC-mass spectra of DMNP (a) UiO-66 in water, pH of 7, in the dark, (b) UiO-66/g-C₃N₄-30% in water, pH of 7 and visible light irradiation



Fig. S10. Stability of catalytic activity over UiO-66/g-C₃N₄-30% at different cycles of reaction



Fig. S11. XRD patterns of UiO-66/g-C₃N₄-30% photocatalyst before and after reaction.

Elements	UiO-66	UiO-66/g-C ₃ N ₄ - 30%
С	47.60	43.18
0	24.38	18.13
Zr	28.02	21.47
Ν	-	17.22
Total	100	100

Table 1S. Element composition of UiO-66 and UiO-66/g-C $_3N_4$ -30% samples.

Table S2. Comparative results of DMNP removal by various heterogeneous materials

Materials	Môi trường, pH	Calculated	Ref.
		t _{1/2} (min)	
UiO-66	N-ethylmorpholine (0.45 M), 10	40	[1]
UiO-66-NH ₂	N-ethylmorpholine (0.45 M), 10	2.8	[2]
PP/ZnO/UiO-66-NH ₂	N-ethylmorpholine (0.45 M), 10	4.80	[3]
Zr-MOFilter UiO-66-NH ₂	N-ethylmorpholine (0.45 M), 10	2.40	[4]
Graphene/UiO-66-NH ₂	N-ethylmorpholine (0.45 M), 10	1.6	[5]
NU-901/branched PEI	N-ethylmorpholine (0.45 M), 10	<u>1.9</u>	[6]
UiO-66	Water, 7	7	[7]
Graphene/UiO-66-NH ₂	Water, 7	60	[5]
UiO-66/g-C ₃ N ₄ -30%	Water, 7	2.17	This
			work

References

- [1] M.J. Katz, J.E. Mondloch, R.K. Totten, J.K. Park, S.T. Nguyen, O.K. Farha, J.T. Hupp, Simple and compelling biomimetic metal-organic framework catalyst for the degradation of nerve agent simulants, Angewandte Chemie - International Edition. 53 (2014). https://doi.org/10.1002/anie.201307520.
- [2] J. Zhao, D.T. Lee, R.W. Yaga, M.G. Hall, H.F. Barton, I.R. Woodward, C.J. Oldham, H.J. Walls, G.W. Peterson, G.N. Parsons, Ultra-Fast Degradation of Chemical Warfare Agents Using MOF–Nanofiber Kebabs, Angewandte Chemie International Edition. 55 (2016). https://doi.org/10.1002/anie.201606656.
- [3] D.T. Lee, J. Zhao, C.J. Oldham, G.W. Peterson, G.N. Parsons, UiO-66-NH2 Metal-Organic Framework (MOF) Nucleation on TiO2, ZnO, and Al2O3 Atomic Layer Deposition-Treated Polymer Fibers: Role of Metal Oxide on MOF Growth and Catalytic Hydrolysis of Chemical Warfare Agent Simulants, ACS Applied Materials and Interfaces. 9 (2017) 44847–44855.

https://doi.org/10.1021/ACSAMI.7B15397/SUPPL_FILE/AM7B15397_SI_001.PDF.

- [4] H. Liang, A. Yao, X. Jiao, C. Li, D. Chen, Fast and Sustained Degradation of Chemical Warfare Agent Simulants Using Flexible Self-Supported Metal-Organic Framework Filters, ACS Applied Materials and Interfaces. 10 (2018) 20396–20403. https://doi.org/10.1021/ACSAMI.8B02886/SUPPL FILE/AM8B02886 SI 001.PDF.
- [5] L. Song, T. Zhao, D. Yang, X. Wang, X. Hao, Y. Liu, S. Zhang, Z.Z. Yu, Photothermal graphene/UiO-66-NH2 fabrics for ultrafast catalytic degradation of chemical warfare agent simulants, Journal of Hazardous Materials. 393 (2020). https://doi.org/10.1016/j.jhazmat.2020.122332.
- [6] Z. Chen, T. Islamoglu, O.K. Farha, Toward Base Heterogenization: A Zirconium Metal-Organic Framework/Dendrimer or Polymer Mixture for Rapid Hydrolysis of a Nerve-Agent Simulant, ACS Applied Nano Materials. 2 (2019) 1005–1008. https://doi.org/10.1021/ACSANM.8B02292/SUPPL FILE/AN8B02292 SI 001.PDF.
- [7] D. Bužek, J. Demel, K. Lang, Zirconium Metal-Organic Framework UiO-66: Stability in an Aqueous Environment and Its Relevance for Organophosphate Degradation, Inorganic Chemistry. 57 (2018). https://doi.org/10.1021/acs.inorgchem.8b02360.