

Highly oxidative GaN:ZnO@ α -Ga₂O₃ heterostructure as a visible-light-driven round-the-clock photocatalyst for dye degradation and disinfection

Yan-Ling Hu,^{*a1} Zihan Zhao,^{b1} Junjie Jiang,^a Yadong Huang,^c Huayu Ji,^a Di Zhu,^a Lianqi Zhang,^a Linhan Zhan,^a Yurong Wu,^a Yuhui Zhang,^a Kun Wu,^a Yun Yang,^d Tian Chai,^{*b} Sujuan Wu,^{*c} Guang-Ling Song^{*c}

^a Fujian Provincial Key Laboratory of Functional Materials and Applications, School of Materials Science and Engineering, Xiamen University of Technology, Xiamen, 361024, China

^b School of Environmental Science & Engineering, Xiamen University of Technology, Xiamen, 361024, China

^c National Engineering Research Center for Magnesium Alloys, College of Materials Science and Engineering, Chongqing University, Chongqing 400044, China

^d Research Institute for Biomimetics and Soft Matter, Fujian Provincial Key Laboratory for Soft Functional Materials Research, Department of Physics, Xiamen University, Xiamen 361005, China

^e Department of Ocean Science and Engineering, Southern University of Science and Technology, Shenzhen, Guangdong 518055, China

*Corresponding authors:

E-mail: huyanling@xmut.edu.cn

Email: chai@xmut.edu.cn

E-mail: sujuan.wu@cqu.edu.cn

E-mail: songgl@sustech.edu.cn

¹Yan-Ling Hu and ¹Zi-Han Zhao contribute equally to this work as the first authors.

E-mail: huyanling@xmut.edu.cn

E-mail: hannazhao7415@163.com

Keywords: Photocatalyst; Round-the-clock; GaN:ZnO; α -Ga₂O₃; Point defects;
Environmental remediation

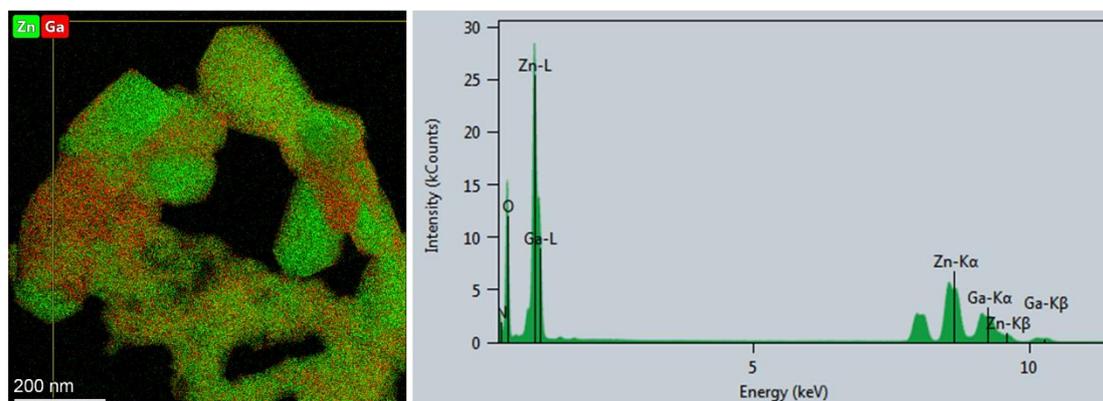


Fig. S1 EDS/STEM mapping for elements Ga and Zn (at. %) and EDS spectrum from the yellow square of Untreated.

Table S1 Compositions of the yellow square in Untreated measured from EDS/STEM

Element	Family	Atomic Fraction (%)
N	K	10.57
O	K	52.83
Zn	K	24.15
Ga	K	12.45

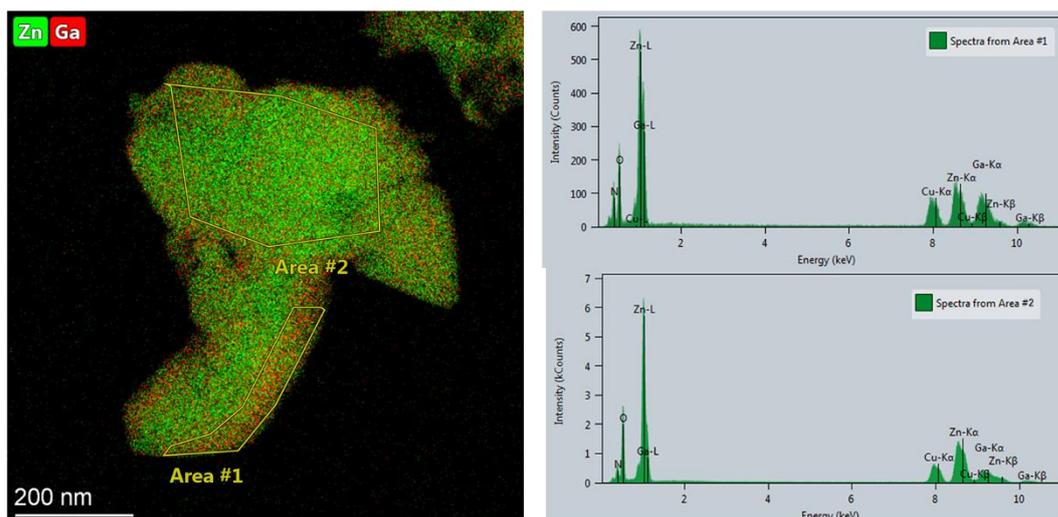


Fig. S2 EDS/STEM mapping for elements Ga and Zn (at. %) and EDS spectrum from two yellow squares of S60.

Table S2 Compositions of the Area 1 in S60 measured from EDS/STEM

Element	Family	Atomic Fraction (%)
N	K	22.64
O	K	37.75
Zn	K	21.74
Ga	K	17.86

Table S3 Compositions of the Area 2 in S60 measured from EDS/STEM

Element	Family	Atomic Fraction (%)
N	K	12.75
O	K	48.49
Zn	K	29.48
Ga	K	9.29

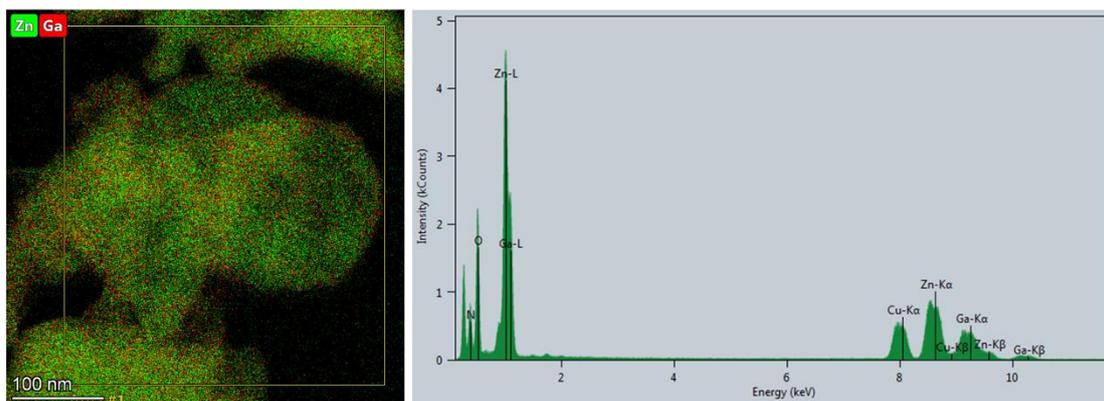


Fig. S3 EDS/STEM mapping for elements Ga and Zn (at. %) and EDS spectrum from the yellow square of S60-HT.

Table S4 Compositions of the yellow square in S60-HT measured from EDS/STEM

Element	Family	Atomic Fraction (%)
N	K	19.42
O	K	45.89
Zn	K	22.61
Ga	K	12.08

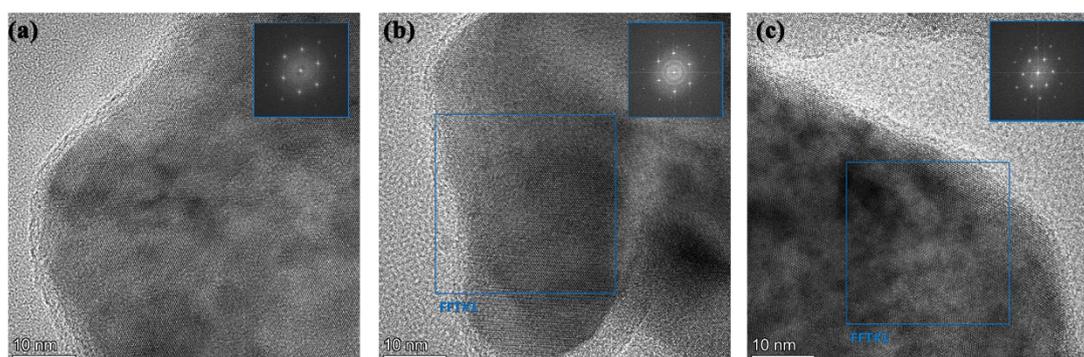


Fig. S4 HRTEM images and the Fast Fourier Transform (FFT) patterns (insets) of (a) Untreated, (b) S60, and (c) S60-HT.

Table S5 Area Ratios for Fitted Peaks in N 1s XPS Spectra

	bonding (binding energy, eV)			
	397.7	396.3	395.8	394.8
	N-H	Ga-N	O _N ...V _{Ga}	Ga LMM
Untreated	0.17	0.30	0.38	0.15
S60	0.25	0.31	0.36	0.08
S60-HT	0.23	0.37	0.37	0.03

Table S6 Area Ratios for Fitted Peaks in Ga 3d XPS Spectra

	bonding (binding energy, eV)					
	V _{Ga}	V _O	Ga-O	Ga-N	Ga-(N-H)	Ga LMM
	(V _O -V _{Ga} /Ga-V _O)					
	21.7	20.7-20.8	20.3	19.7-19.8	19.1	18.5
Untreated	0	0.08	0.06	0.43	0.35	0.08
S60	0	0.19	0.11	0.37	0.31	0.02
S60-HT	0.03	0.18	0.10	0.39	0.30	0

Table S7 Area Ratios for Fitted Peaks in O 1s XPS Spectra

	bonding (binding energy, eV)		
	532.4-533.0	531.3-531.9	530.3-530.7
	O _{ad}	Zn(Ga)-V _O	Zn(Ga)-O
Untreated	0.27	0.32	0.41
S60	0.19	0.50	0.31
S60-HT	0.32	0.51	0.17

Table S8 Area Ratios for Fitted Peaks in Zn 2p XPS Spectra

	bonding (binding energy, eV)			
	1023	1022.5	1021.7	1021
	V _{Zn...Ga_{Zn}}	Zn-V _O	Zn-O	O _{N...V_{Ga}}
Untreated	0.07	0.03	0.43	0.47
S60	0.12	0.34	0.24	0.30
S60-HT	0.21	0.22	0.30	0.27

Table S9 Area Ratios for Fitted Peaks in O 1s XPS Spectra of S60-HT

	bonding (binding energy, eV)		
	533	531.7	530.7-530.8
	O _{ad}	Zn(Ga)-V _O	Zn(Ga)-O
dark	0.41	0.53	0.06
light	0.58	0.33	0.09

Table S10 Area Ratios for Fitted Peaks in Ga 3d XPS Spectra of S60-HT

	bonding (binding energy, eV)				
	V _{Ga}	V _O	Ga-O	Ga-N	Ga-(N-H)
	21.7	20.8	20.3	19.8	19.1
dark	0.03	0.51	0.08	0.31	0.07
light	0.03	0.42	0.14	0.33	0.08

Table S11 Area Ratios for Fitted Peaks in Zn 2p XPS Spectra of S60-HT

	bonding (binding energy, eV)			
	1023.1	1022.3	1021.5	1020.5
	V _{Zn} ...Ga _{Zn}	Zn-V _O	Zn-O	Zn-O _N ...V _{Ga}
dark	0.17	0.44	0.33	0.06
light	0.18	0.51	0.25	0.06

Table S12 Area Ratios for Fitted Peaks in N 1s XPS Spectra of S60-HT

	bonding (binding energy, eV)		
	398.5	397.0	395.7
	N-H	Ga-N	O _N ...V _{Ga}
dark	0.23	0.30	0.47
light	0.29	0.28	0.43