Electronic Supplementary Material (ESI) for Environmental Science: Nano.

Electronic Supplementary Information

Unveiling the Origin of Efficient Photocatalytic Degradation of Nitazoxanide Over Bismuth (Oxy)Iodide Crystalline Phases

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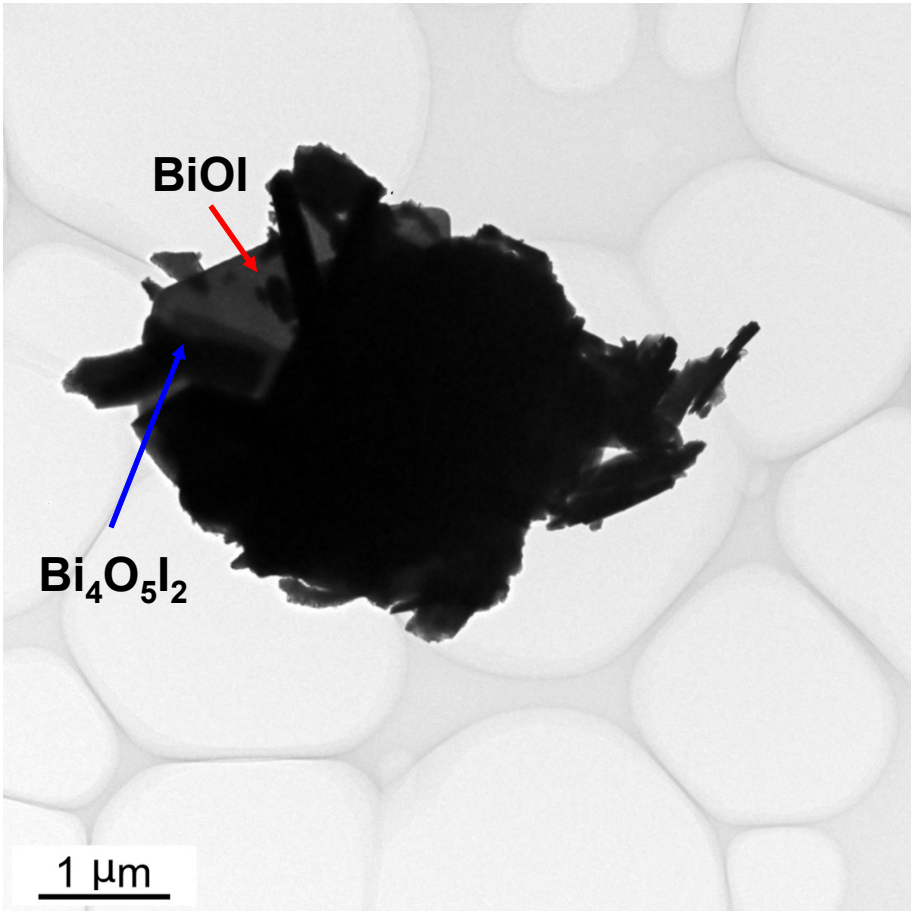

Figure S1. TEM image of BiOI/$Bi_4O_5I_2$ heterostructures.

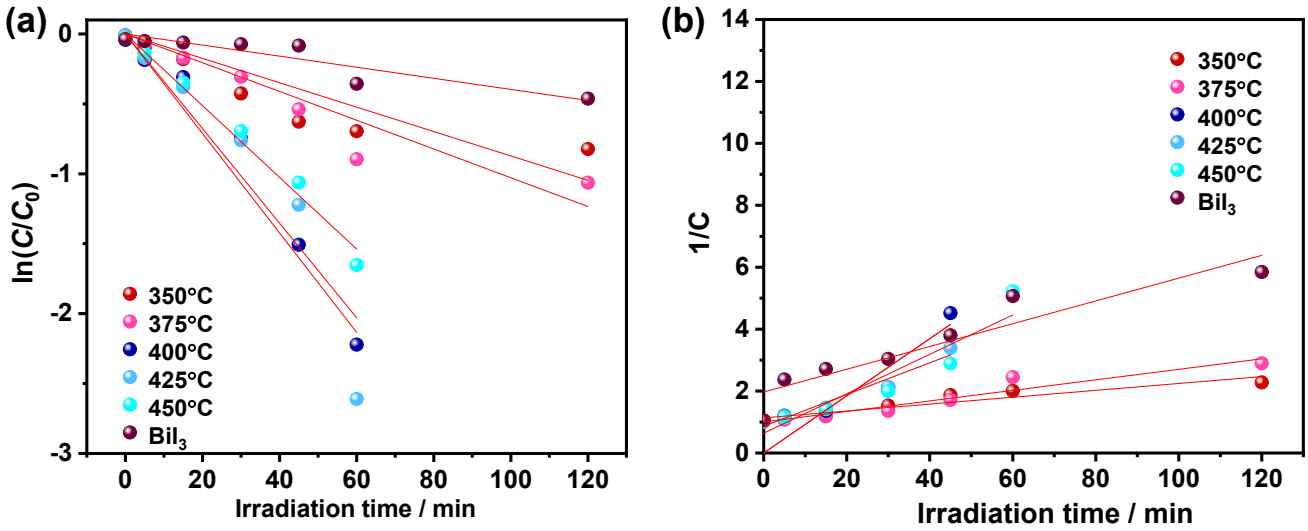

Figure S2. Comparison of pseudo-first-order (a) and pseudo-second-order (b) kinetic models of the photocatalytic removal of nitazoxanide by the synthesized photocatalysts.

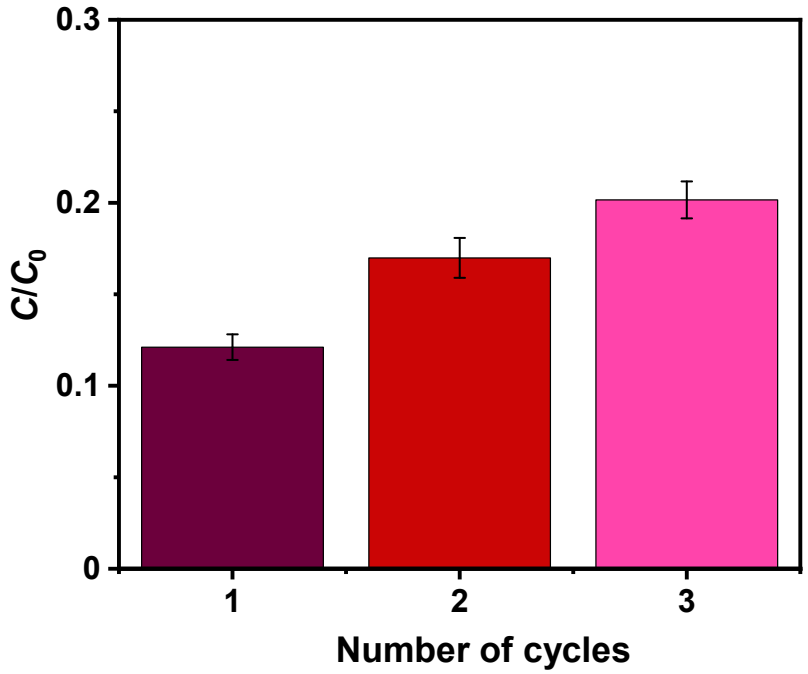

Figure S3. Reusability test of the sample thermally treated at 375°C for the photocatalytic degradation of nitazoxanide for three consecutive cycles.

Table S1. Comparison of efficiencies of bismuth oxyiodides for the removal of carious pollutants.

Photocatalyst	Pollutant	Conditions	Efficiency	Ref.
$BiOI/Bi_4O_5I_2$ (375)	Nitazoxanide	Under visible light irradiation	100%, 60 min	*This study*
$BiOI/Bi_4O_5I_2$ (400)	Methylene blue	Under visible light irradiation	100%, 120 min	*Inorg. Chem. Commun.*, 2018, **93**, 65–68.
$ZnFe_2O_4$/BiOI/AgI	Rhodamine B	Under visible light irradiation	100%, 90 min photocatalysis 100%, 35 min photo-Fenton	*Mater. Res. Bull.*, 2024, **169**, 112508.
Ag-BiOI	Diclofenac sodium	Photoelectrocatalysis	92%, 240 min	*Sci. Rep.*, 2022, **12**, 4214
BiOI/UiO-66 p-n heterojunction	Sulfadiazine	Under visible light irradiation	100%, 90 min	*Chem. Eng. J.*, 2023, **451**, 138624.
BiOI	Sulfamethoxazole	Under visible light irradiation	<80%, 60 min photocatalysis 100%, 30 min in combined with chlorination	*Chem. Eng. J.*, 2023, **452**, 139103.
$BiOBr_xI_{(1-x)}$	Rhodamine B, tetracycline hydrochloride	Under visible light irradiation	100% RhB, 12 min 90% TCH, 12 min	*Mater. Res. Bull.*, 2024, **169**, 112506.
BiOI/BiOBr	Tetracycline	Under visible light irradiation	90%, 90 min	*Appl. Catal. B*, 2024, **304**, 123226.
BiOI/NH_2-MIL125(Ti)	Oxytetracycline	Photocatalytic-ozonation	100%, 100 min	*Sci. Rep.*, 2023, **13**, 11113
$Bi_3O_4Cl/Bi_4O_5I_2$	Tetracycline, Rhodamine B	Under visible light irradiation	70.6% TC, 60 min 97.4% RhB, 60 min	*J. Colloid Interface Sci.*, 2023, **652**, 798–812.
$Ag/Bi_4O_5I_2$/ reduced graphene oxide	Tetracycline hydrochloride, ofloxacin, levofloxacin	Under visible light irradiation	90.2% TCH 60.9% ofloxacin 38.5% for levofloxacin after 180 min	*Mater. Today Sustain.*, 2023, **24**, 100478.

Table S2. Adsorption energy of nitazoxanide and water molecules.

Crystal plane	E_{ads} (kcal·mol^{-1})	dE_{ads}/dN_i (*nitazoxanide*)	dE_{ads}/dN_i *(water)*
BiOI (1 0 2)	-138.92	-64.51	-6.69
BiOI (1 1 0)	-124.54	-69.28	-5.18
BiOI ($1\bar{1}0$)	-122.20	-68.43	-4.85
$Bi_4O_5I_2$ ($\bar{1}01$)	-46.81	-25.17	-0.03
BiOI (1 1 0) + $Bi_4O_5I_2$ ($\bar{1}01$)	-121.52	-66.71	-5.07
BiOI (1 0 2) + $Bi_4O_5I_2$ ($\bar{1}01$)	-147.10	-65.87	-7.59
Bi_5O_7I (2 0 0)	-43.61	-24.76	-1.63
BiI_3 ($2\bar{1}3$)	-42.94	-22.63	-0.07