Polyaniline enhances the visible light photocatalytic activities of bismuth oxyhalides

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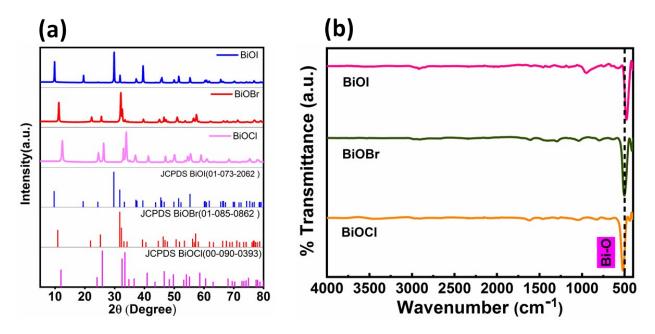


Fig. S1 (a) XRD pattern and (b) FTIR spectra of as synthesized BiOX.

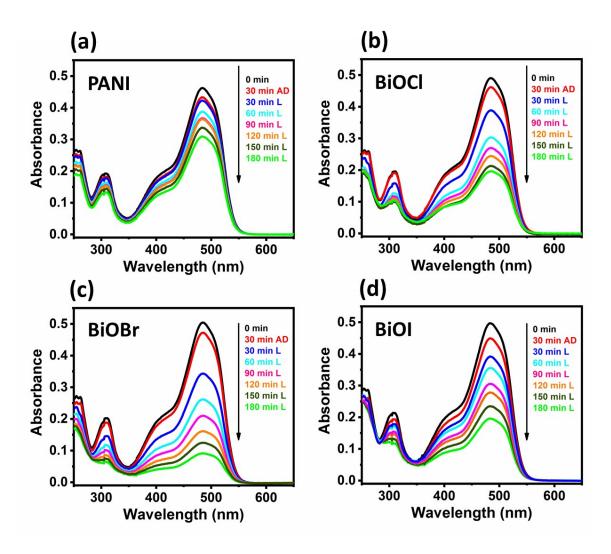


Fig. S2 UV-vis absorbance spectra of photocatalytic OII dye degradation under visible light for : (a) PANI, (b) BiOCl, (c) BiOBr, and (d) BiOI photocatalyst.

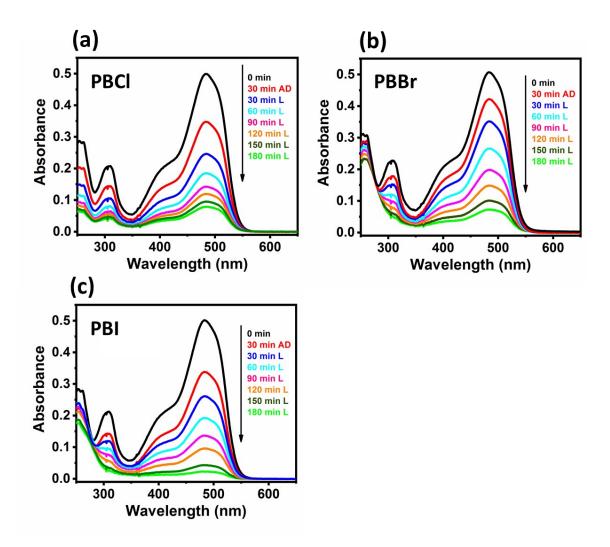


Fig. S3 UV-vis absorbance spectra of photocatalytic OII dye degradation under visible light for : (a) PBCl, (b) PBBr, and (c) PBI composite photocatalyst.

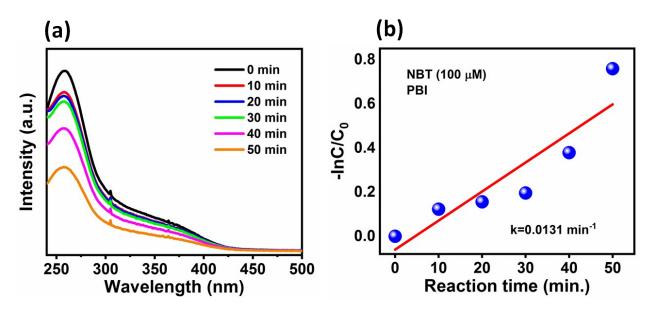


Fig. S4 (a) Time-resolved UV-visible absorbance spectra of NBT during visible light irradiation in presence of PBI composite and (b) the respective kinetic curve.

Concentration of •O₂⁻ radicals was calculated using the formula:

Concentration of $\bullet O_2^-$ radical = $\mathbf{k}_{NBT} \times \mathbf{t} \times \mathbf{C}_{initial} \times \mathbf{4}$

 $k_{NBT} = 0.0131 \text{min}^{-1} \text{ (loss kinetic constant of NBT)}$

t = 50 min (the light exposure time)

 $C_{initial} = 100 \mu M \text{ (NBT initial concentration)}$

4 is the constant coefficient between the reaction of NBT and •O₂⁻

Concentration of ${}^{\bullet}O_2^-$ radical = 2.62×10^{-5} M

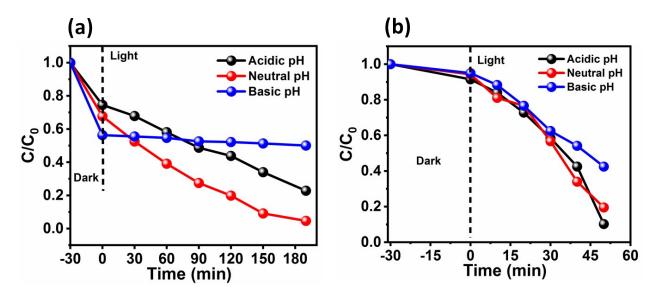


Fig. S5 Effect of varying pH (acidic, 0.1 M HCl neutral and basic, 0.1 M NaOH) on the photocatalytic performance of PBI on (a) degradation of OII dye, and (b) photocatalytic reduction of Cr(VI) to Cr(III).

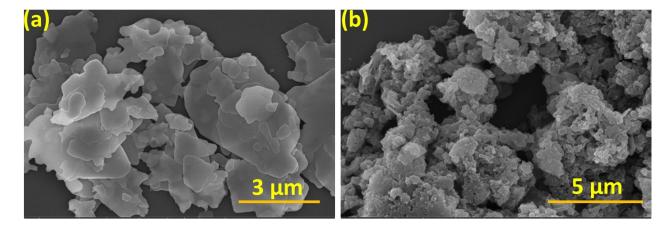


Fig. S6 FESEM images of (a) BiOI and (b) PANI

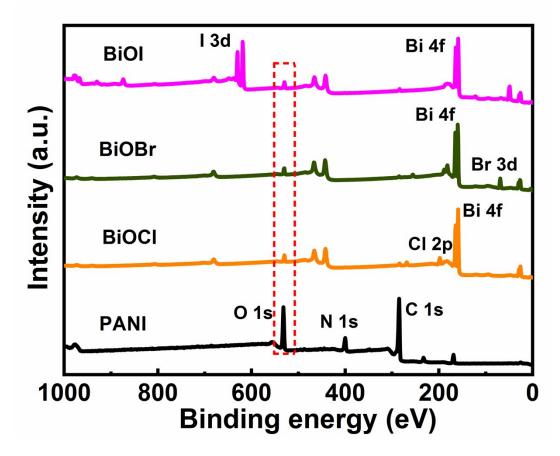


Fig. S7 XPS survey spectrum of PANI and as synthesized nanocomposites

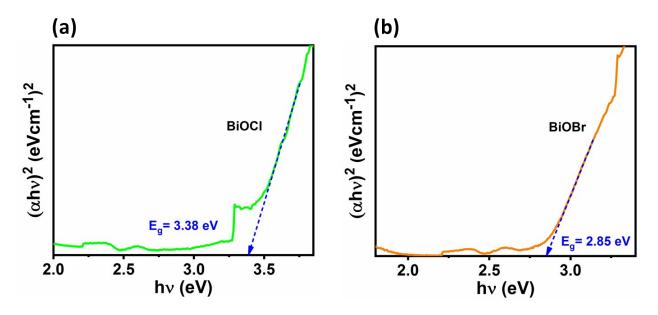


Fig. S8 Tauc plot showing band gap enegy of (a) BiOCl and (b) PANI BiOBr.

Table: S1 Comparison of the photocatalytic activity of the PANI-BiOI with some other hybrid composites for the degradation of various pollutants under visible light.

Photocatalyst	Pollutant, Conc. (ppm)	Catalyst amount (mg/mL)	Light source	Removal (%)	Time (min)	Ref.
ZnO/BiOI	MO, 10	1	Halogen tungsten lamp (500 W)	78	240	1
BiOI/Bi ₂ MoO ₆	RhB, 7	1	Xe lamp (300 W)	95	90	2
2D/3D g-C ₃ N ₄ /BiOI	AR, 10	0.1	Mercury lamp (250 W)	74.64	150	3
Ppy-BiOI	RhB, 4 BPA, 30 2,4-DCP, 30 TC, 30	1 1 1 1	Xe lamp	83 50 29 61	300 300 300 300	4
AgI/BiOI	MO, 20 Phenol, 20	1	Xe lamp (300 W)	90.2 41.6	180 180	5
BiOI/BiVO ₄	RhB, 5	0.6	Xe lamp (300 W)	97	75	6
NiS/BiOI	RhB, 20 TC, 50 Cr(VI), 50	0.3 0.3 0.27	Xe lamp (300 W)	99.8 96.3 92.8	200 140 180	7
Fe-nPPy/BiOI	CV, 10 TC, 20	0.5	White LED (192 W)	84 74	120 120	8
PANI/BiOI	OII, 20 Cr(VI)	0.5 0.5	White LED (160 W)	95.3 90	180 50	Current work

References:

- 1 J. Jiang, X. Zhang, P. Sun and L. Zhang, 2011, 20555–20564.
- 2 Y. Wang, M. Wang, J. Liu, L. Wang, H. Pang, Y. Su, J. Pan, Z. Z. Xue and Y. Peng, *Inorg. Chem.*, 2023, **62**, 9158–9167.
- 3 J. Li, L. Guan, L. Jiang, M. Xu, J. Li, J. Zuo, C. Tan and Z. Xia, *ACS Omega*, 2024, **9**, 361–370.
- 4 J. Xu, Y. Hu, C. Zeng, Y. Zhang and H. Huang, J. Colloid Interface Sci., 2017, **505**, 719–727.
- 5 H. Cheng, B. Huang, Y. Dai, X. Qin and X. Zhang, *Langmuir*, 2010, **26**, 6618–6624.
- 6 S. Ni, T. Zhou, H. Zhang, Y. Cao and P. Yang, ACS Appl. Nano Mater., 2018, 1, 5128–5141.

- 7 C. T. Haile, N. Ahmad, C. W. Chiu and C. F. Jeffrey Kuo, *Chemosphere*, 2023, **323**, 138108.
- 8 R. Kumar, R. Gogoi, K. Sharma, A. Singh and P. F. Siril, *Environ. Sci. Adv.*, 2023, **3**, 85–96.