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

Facile Synthesis of Z-Scheme Fe-nPPy/BiOI Nanocomposite for Enhanced Visible Light Driven Photocatalytic Activity

Rajesh Kumar[a,b], Rituporn Gogoi[a], Kajal Sharma[a], Astha Singh[a], Prem Felix Siril[a]*

[a] School of Chemical Sciences, Indian Institute of Technology Mandi, Mandi, Himachal Pradesh-175005, India
[b] Govt. College Kullu, Himachal Pradesh- 175101, India
*Corresponding author: prem@iitmandi.ac.in

Table of Content:

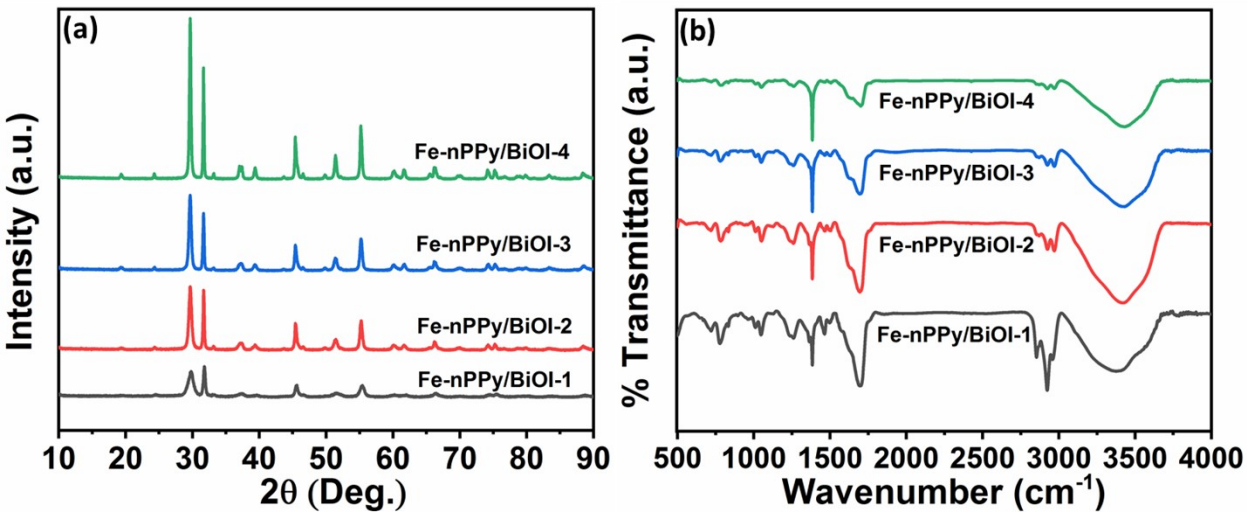

Fig. S1: (a) XRD patterns and (b) FTIR spectra of the synthesized nanocomposites.

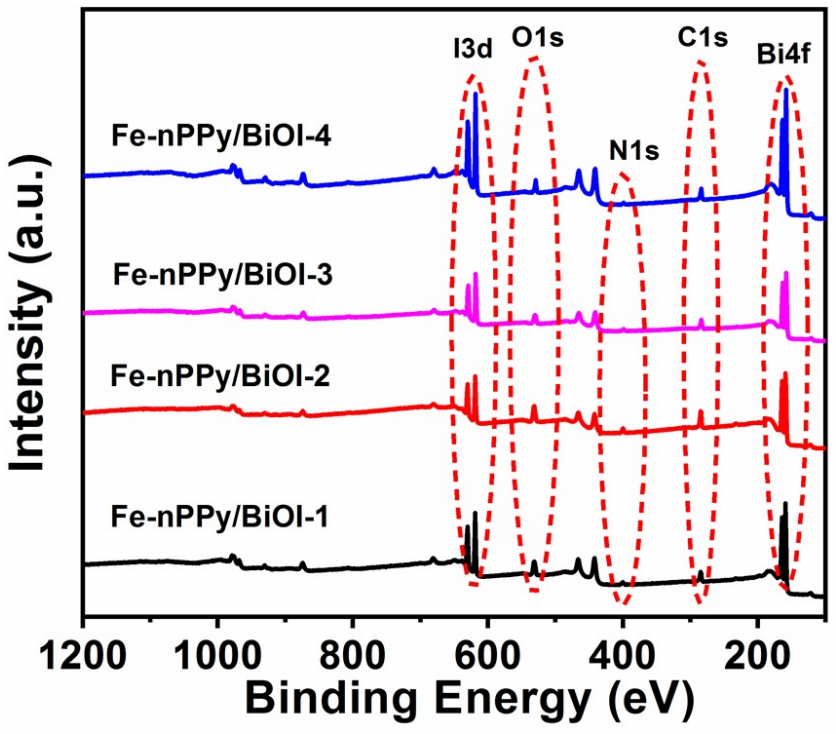

Fig. S2: XPS survey spectra of as synthesized nanocomposites.

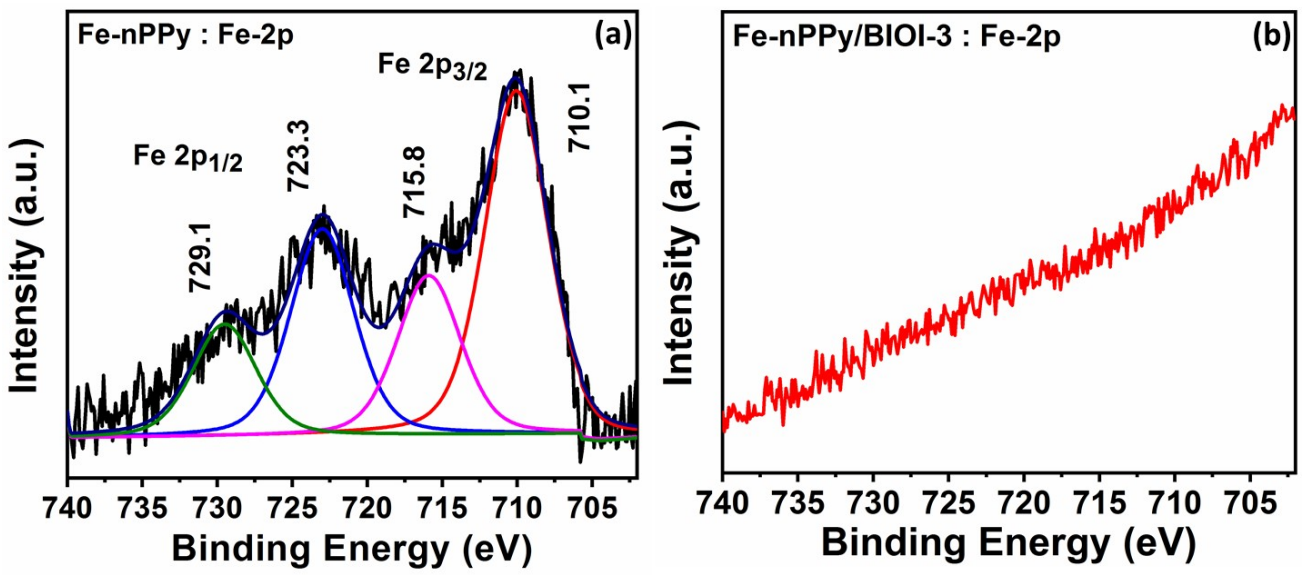

Fig. S3: Deconvoluted Fe2p XPS spectra of (a) Fe-nPPy and (b) Fe-nPPy/BiOI-3.

Table S1: Surface elemental composition of Fe-nPPy/BiOI-3 as per XPS survey spectra.

Name	Peak BE	FWHM eV	Area (P) CPS.eV	Atomic %	Q	SF
I3d	619.75	1.58	2755213.41	7.27	1	42.416
Bi4f	159.88	2.52	5469514.21	11.55	1	38.304
C1s	285.87	3.08	608732.95	53.19	1	1
O1s	531.23	4.23	596396.4	21.53	1	2.881
N1s	400.79	3.3	110187.25	6.2	1	1.676
Fe2p	720.08	0.56	29798.18	0.25	1	14.353

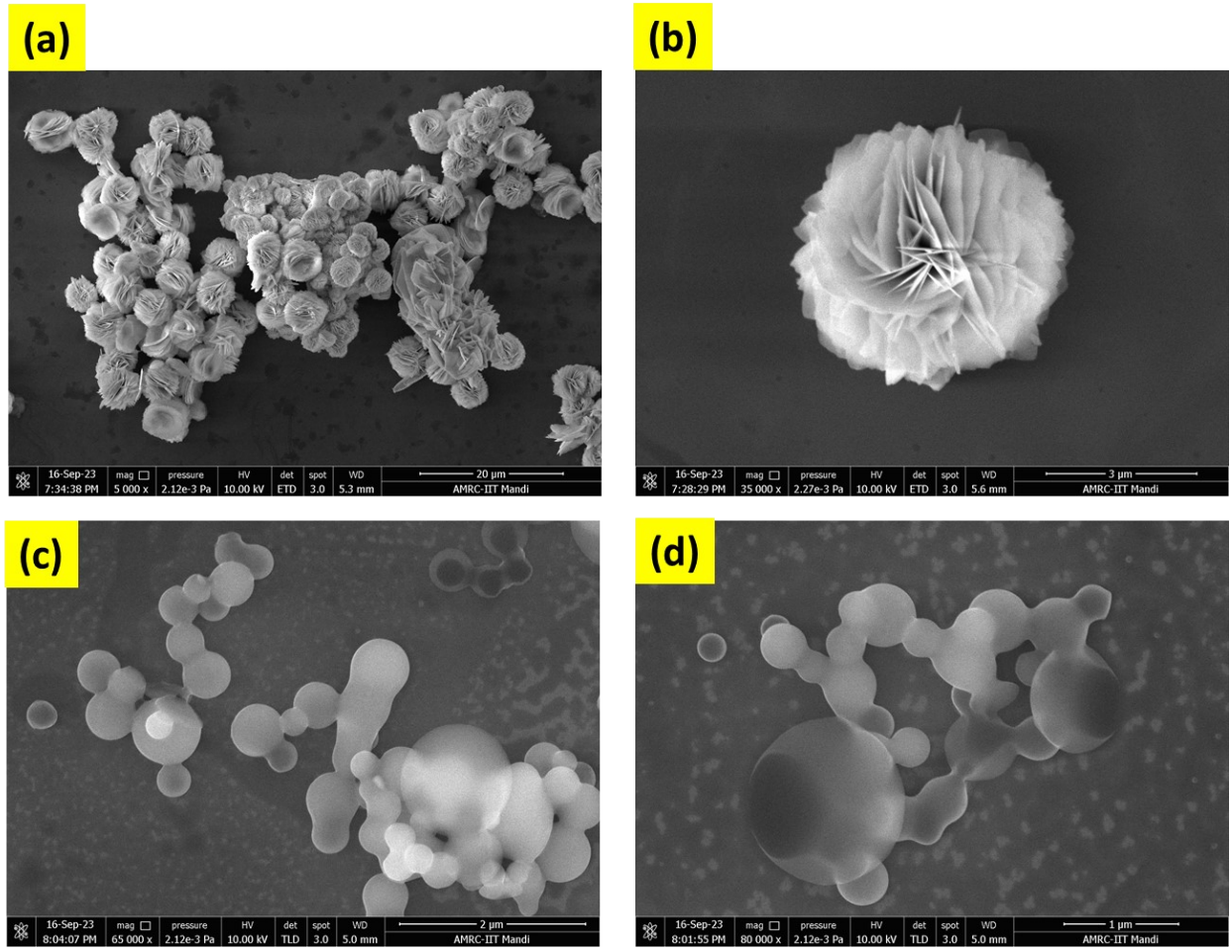

Fig. S4: FESEM images of: (a & b) BiOI and (c & d) Fe-nPPy.

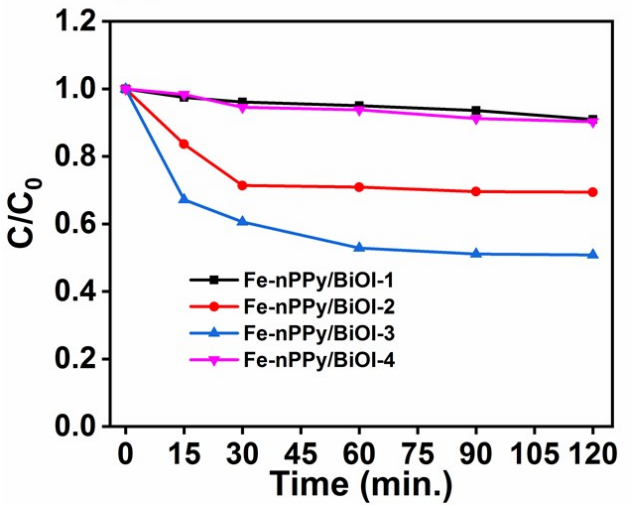

Fig. S5: (a) Adsorption profiles of CV dye over Fe-nPPy/BiOI catalysts.

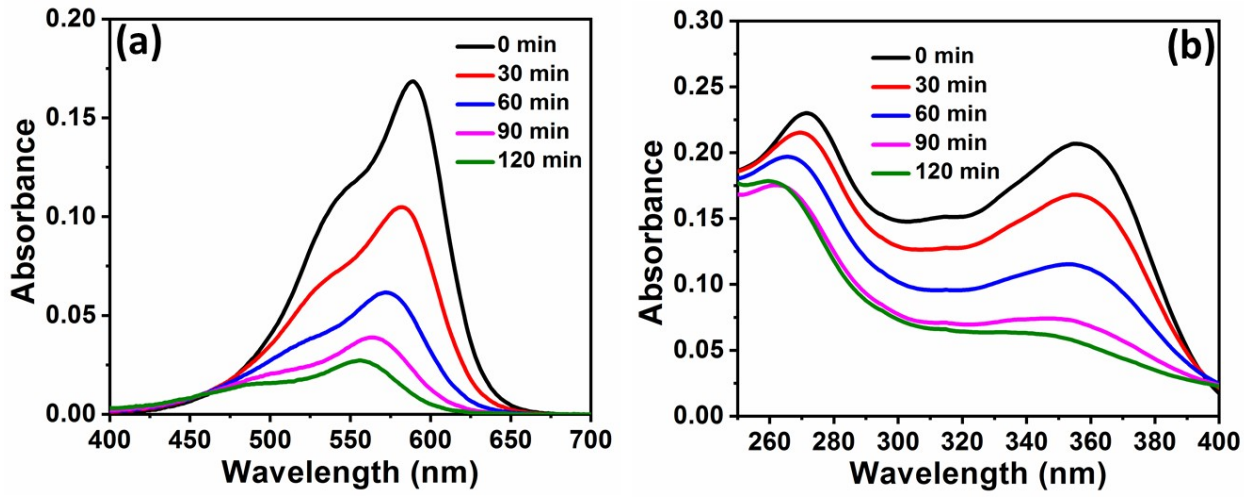

Fig. S6: Variation in the UV-Vis absorbance spectra with time of: (a) CV dye and (b) Tetracycline (TC) using Fe-nPPy/BiOI-3 photocatalyst under visible light irradiation.

Table S2: Comparison of the photocatalytic activity of the Fe-nPPy/BiOI-3 with some other hybrid composites for the degradation of Crystal violet (CV) dye and Tetracycline (TC) under visible light irradiation.

Photocatalyst	**Pollutant, concentration (ppm)**	**Catalyst amount (mg/mL)**	**Visible light source**	**Synthesis method**	**Removal (%)**	**Time (min.)**	**References**
g-C_3N_4/Ag_3VO_4	CV, 20	1	500 W Xe arc lamp	ultrasound-assisted	85	150	[1]
F-TiO_2(B)/ fullerene	CV, 30	0.1	500 W halogen lamp	Ballmill + hydrothermal	77.2	120	[2]
$SrFeO_3$−x/g-C_3N_4	CV, 10	0.1	150 W Xe arc lamp	sintering method	99.9	720	[3]
Gd doped $BiFeO_3$	CV, 20	0.2	250 W mercury lamp	auto-combustion method	84.5	150	[4]
Fe-nPPy/BiOI-3	CV, 10	0.5	192 W white LEDs	RT co-precipitation	84.0	120	Current work
Fe_3O_4@TiO_2–Co	TC, 50	0.2	300 W Xe lamp	Facile reduction method	92.4	120	[5]
Ag/AgBr/AgI@ SiO_2 aerogel	TC, Not known	0.3	300 W Xe arc lamp	Supercrictical drying process	79.5	50	[6]
PPy-BiOI	TC, 30	1	Not known	Co-precipitation	61	300	[7]
Fe-nPPy/BiOI-3	TC, 20	1	192 W white LEDs	RT co-precipitation	74	120	Current work

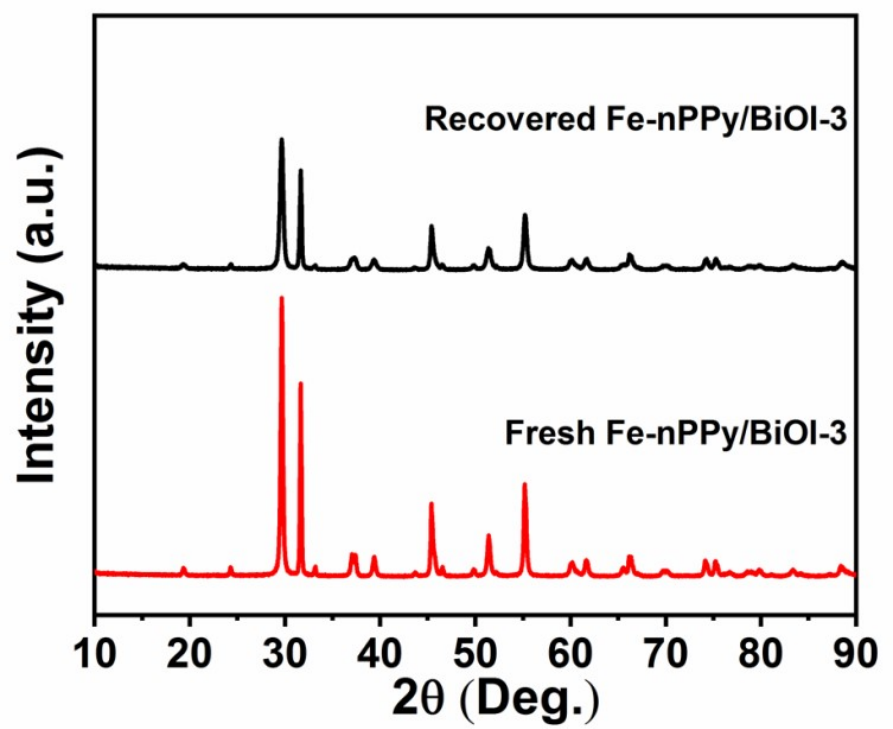

Fig. S7: XRD patterns of fresh and recovered Fe- nPPy/BiOI-3 photocatalyst after three cycles

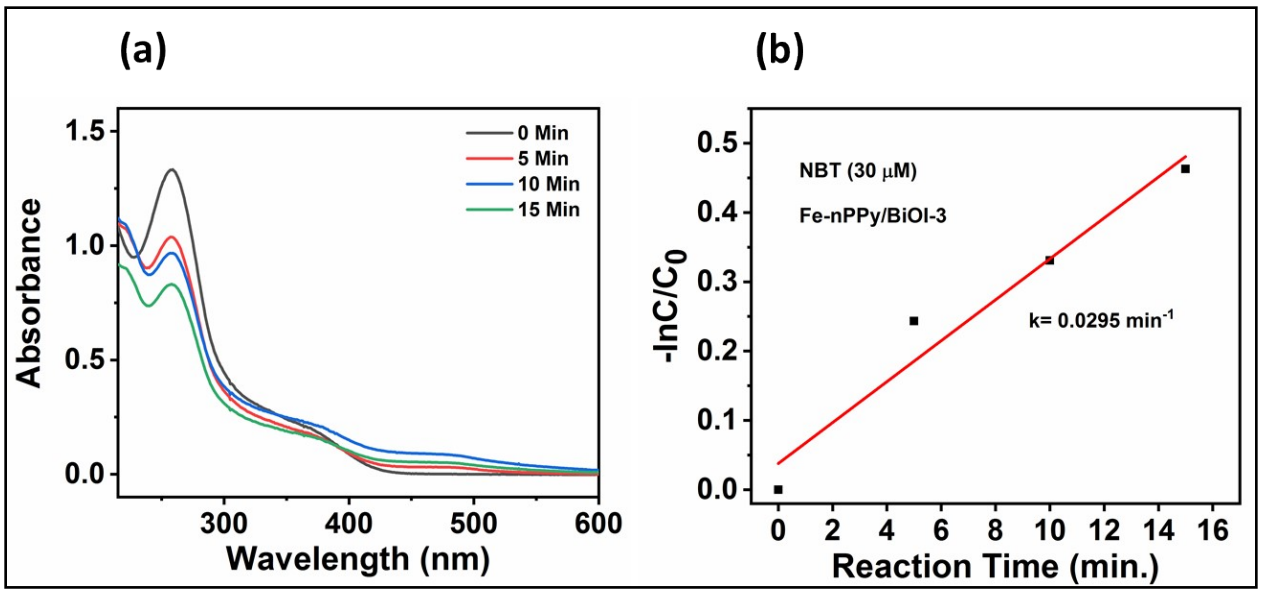

Fig. S8: (a) Time-dependent variation of the UV-visible absorbance spectra of NBT during visible light irradiation in presence of Fe-nPPy/BiOI-3 photocatalyst and (b) the respective kinetic curve.

Concentration of $\bullet O_2^-$ radical = $k_{NBT} \times t \times C_{initial} \times 4$

k_{NBT} = 0.0295 min^{-1} (loss kinetic constant of NBT)

t = 15 min (the light exposure time)

$C_{initial}$ = 30 μM (NBT initial concentration)

4 is the constant coefficient between the reaction of NBT and $\bullet O_2^-$

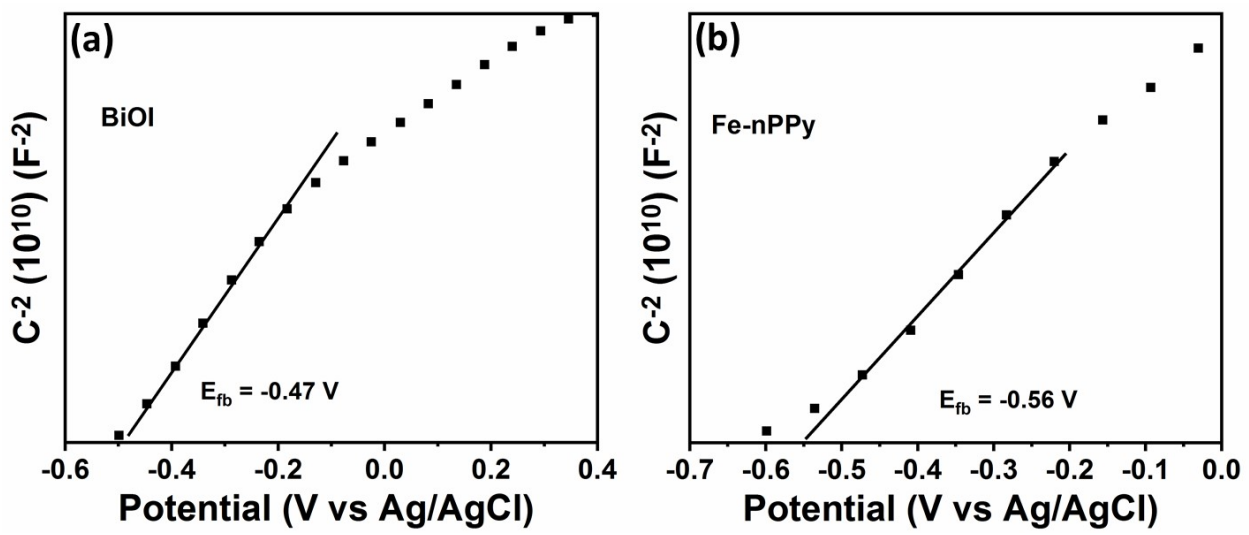

Fig. S9: (a) Mott-Schottky plots of (a) BiOI and (b) Fe-nPPy.

We have used the following relation for conduction band calculation;

E (RHE) = E (Ag/AgCl) + 0.197 (at pH = 7)

Further, valence band edge is calculated by applying the relation;

$E_{CB} = E_{VB} - E_g$ (E_g is calculated from DRS studies for BiOI and Fe-nPPy)

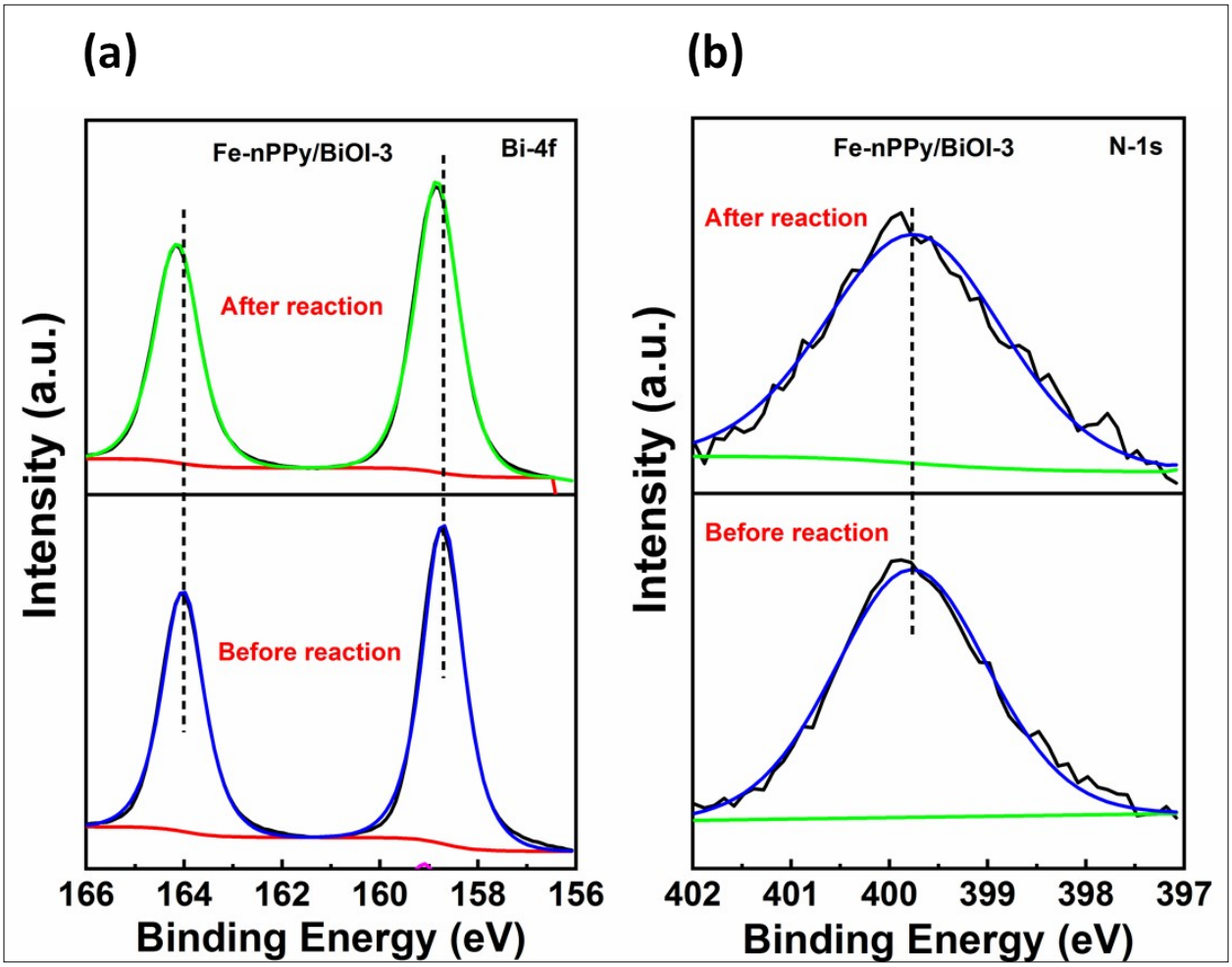

Fig. S10: XPS spectra of Fe-nPPy/BiOI-3 before and after photocatalysis for Bi-4f and N-1s respectively.

References:

S[1]: S. Wang, D. Li, C. Sun, S. Yang, Y. Guan, H. He, Synthesis and characterization of g-C3N4/Ag3VO4 composites with significantly enhanced visible-light photocatalytic activity for triphenylmethane dye degradation, Appl. Catal. B Environ. 144 (2014) 885–892. https://doi.org/10.1016/j.apcatb.2013.08.008

S[2]: Y. Panahian, N. Arsalani, R. Nasiri, Enhanced photo and sono-photo degradation of crystal violet dye in aqueous solution by 3D flower like F-TiO2(B)/fullerene under visible light, J. Photochem. Photobiol. A Chem. 365 (2018) 45–51. https://doi.org/10.1016/J.JPHOTOCHEM.2018.07.035

S[3]: H.P. Lin, C.C. Chen, W.W. Lee, Y.Y. Lai, J.Y. Chen, Y.Q. Chen, J.Y. Fu, Synthesis of a SrFeO3-x/g-C3N4 heterojunction with improved visible-light photocatalytic activities in chloramphenicol and crystal violet degradation, RSC Adv. 6 (2016) 2323–2336. https://doi.org/10.1039/c5ra21339h

S[4]: S. Kossar, I.B.S. Banu, N. Aman, R. Amiruddin, Investigation on photocatalytic degradation of crystal violet dye using bismuth ferrite nanoparticles, J. Dispers. Sci. Technol. 42 (2021) 2053–2062. https://doi.org/10.1080/01932691.2020.1806861

S[5]: Tan, Q., Zhang, W., ... Niu, Li, 2023. Magnetically induced construction of core-shell architecture Fe3O4@TiO2-Co nanocomposites for effective photocatalytic degradation of tetracycline. New Journal of Chemistry 47, 15951–15962. doi:10.1039/d3nj02080k

S[6]: Ma, C., Shi, F., Liu, J., Li, T., Zhu, K., Liu, J., … Xiao, J. (2023, June 1). Construction of a novel Ag/AgBr/AgI@SiO2 composite aerogel with controlled pore structure: Efficient removal of tetracycline by adsorption/photocatalysis synergism under visible light irradiation. Journal of Environmental Chemical Engineering. Elsevier Ltd. https://doi.org/10.1016/j.jece.2023.110157

S[7]: Xu, J., Hu, Y., Zeng, C., Zhang, Y., & Huang, H. (2017). Polypyrrole decorated BiOI nanosheets: Efficient photocatalytic activity for treating diverse contaminants and the critical role of bifunctional polypyrrole. Journal of Colloid and Interface Science, 505, 719–727. https://doi.org/10.1016/j.jcis.2017.06.054