Electronic Supporting Information (ESI)

$BiFe_{0.5}Cr_{0.5}O_3$ Nanocatalysts for Sustainable Solar-Light-Driven Purification of Pharmaceutical Wastewater†

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Sample preparation

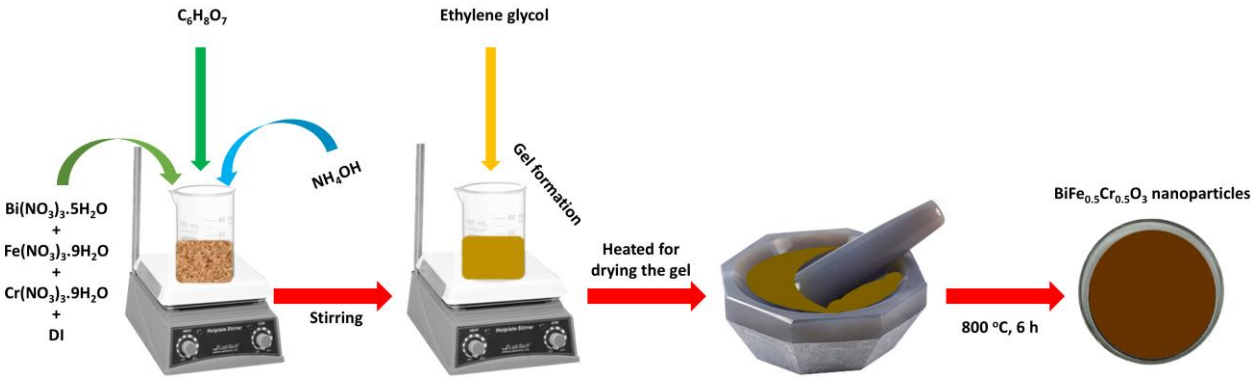

Fig. S1. *Schematic representation of the synthesis procedure of porous $BiFe_{0.5}Cr_{0.5}O_3$ nanoparticles by sol-gel technique.*

$BiFe_{0.5}Cr_{0.5}O_3$ (BFCO) perovskite nanoparticles were synthesized via a sol-gel approach, as illustrated in Fig. S1 [1,2]. Precisely measured amounts of bismuth nitrate pentahydrate, iron nitrate nonahydrate, and chromium nitrate nonahydrate were each dissolved in 100 mL of deionized water and stirred for 15–20 minutes to ensure complete dissolution. The solutions were then combined, and citric acid was introduced as a chelating agent to stabilize metal ions and prevent premature precipitation. The pH was adjusted to 7 by gradually adding ammonium hydroxide, creating an optimal neutral environment. Ethylene glycol was then incorporated to

facilitate gel formation by promoting a polymeric network of metal cations. The solution was maintained at room temperature for four hours before being heated to 200 °C, initiating combustion that decomposed organic components and generated metal oxides in powder form. This combustion process was carefully controlled to ensure complete removal of organic residues. The resulting material was finely ground with an agate mortar to achieve uniformity before undergoing calcination at 800 °C for six hours at a heating rate of 5 °C per minute.

Electrochemical cell setup

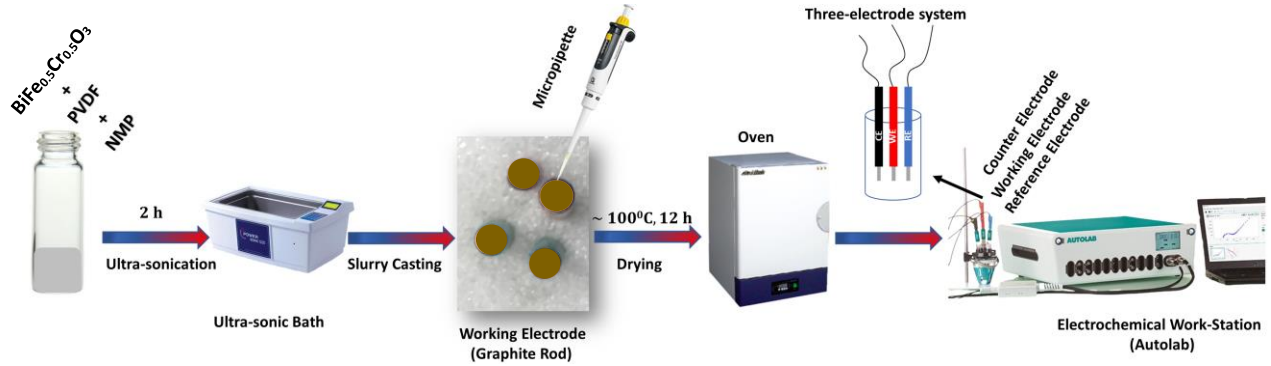

Fig. S2 *Schematic illustration of the preparation of electrode slurry and the configuration of the electrochemical setup.*

A three-electrode system was utilized with a 1 M Na_2SO_4 aqueous solution as the electrolyte [2,3]. The reference electrode was an Ag/AgCl electrode immersed in a saturated 3.5 M KCl solution, while a platinum wire served as the counter electrode. For the working electrode preparation, 20 mg of $BiFe_{0.5}Cr_{0.5}O_3$ nanoparticles (90 wt%) were mixed with 2.22 mg of polyvinylidene fluoride (PVDF, 10 wt%) as a binder and 200 µL of N-methyl-2-pyrrolidone (NMP) as the solvent. The mixture was sonicated for 2 hours to ensure a uniform slurry. This slurry was then carefully applied to a graphite rod with a surface area of 0.28 cm^2. Afterward, the coated graphite rod was dried at 100°C for 12 hours to remove the solvent and ensure proper bonding of the active material. This modified graphite rod was then employed as the working electrode for electrochemical and photoelectrochemical such as cyclic voltammetry (CV), linear sweep voltammetry (LSV), Mott-Schottky, and electrochemical impedance spectroscopy (EIS) analysis.

Experimental setup for photocatalytic degradation of pollutants from water

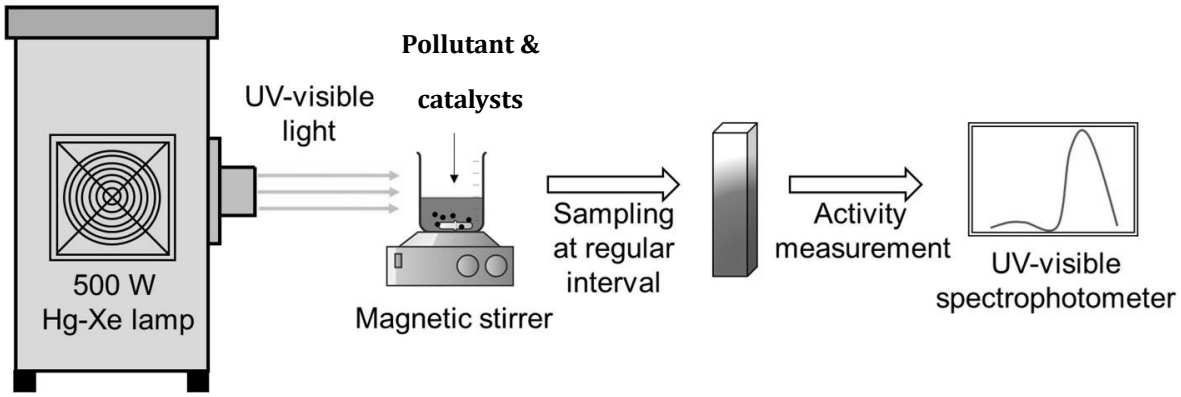

Fig. S3. *Schematically a photocatalytic reactor setup for the pollutant degradation experiments. Irradiation power density was 100 mW cm^{-2}.*

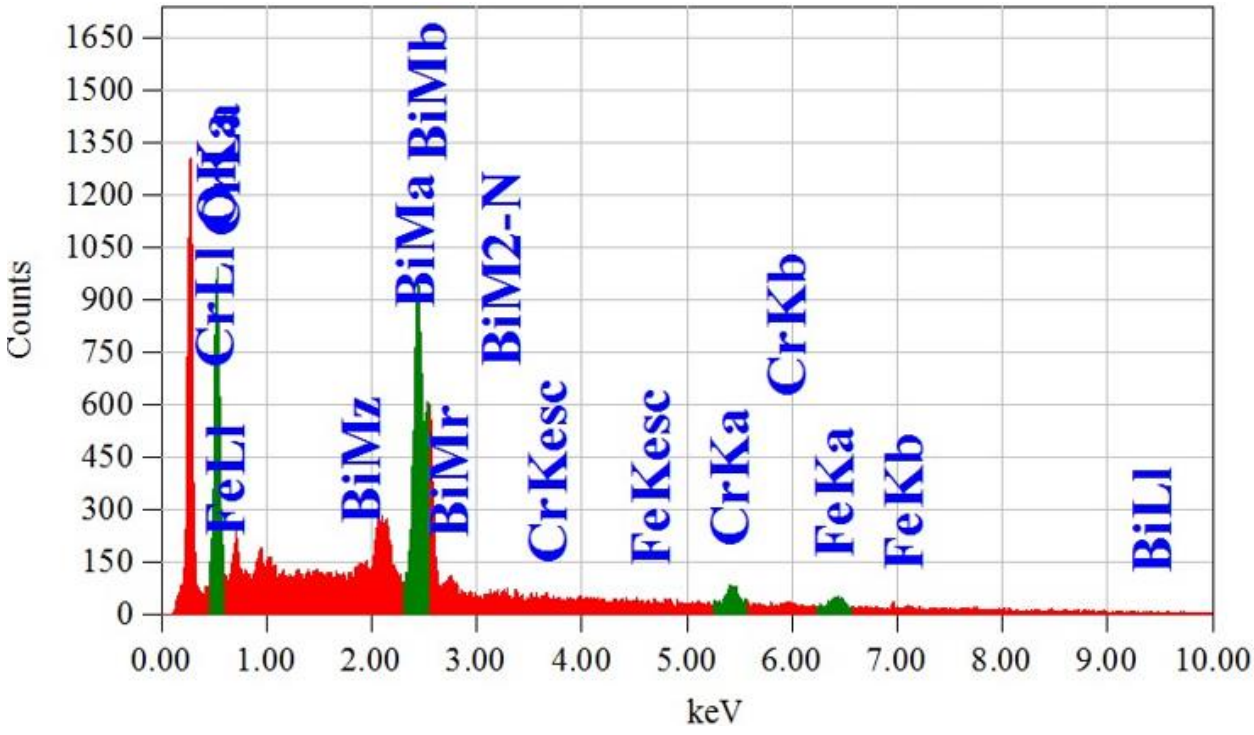

Fig. S4. *Energy Dispersive X-ray (EDX) spectra of $BiFe_{0.5}Cr_{0.5}O_3$ nanoparticles.*

Table S1 *Mass and atomic percentages of corresponding elements in $BiFe_{0.5}Cr_{0.5}O_3$ nanoparticles as obtained via EDX analysis were consistent with theoretical analysis, which indicates the successful formation of $BiFe_{0.5}Cr_{0.5}O_3$ nanoparticles.*

Elements	Mass (%) (theoretical)	Mass (%) (experimental)	Atom (%) (theoretical)	Atom (%) (experimental)
Bi	67.22	66.91	20	20.08
Fe	8.98	9.19	10	10.32
Cr	8.36	8.87	10	10.70
O	15.44	15.03	60	58.91

Table S2 *The XPS spectrum of $BiFe_{0.5}Cr_{0.5}O_3$ nanoparticles revealed several distinct peaks corresponding to the oxidation states of Bi, Fe, Cr and O.*

Element	Orbital	Peaks	Binding energy (eV)
Bi	Bi 4f	$4f_{7/2}$ (Bi^{3+})	163.82
		$4f_{5/2}$ (Bi^{3+})	158.51
Fe	Fe 2p	satellite	733.71
		$2p_{3/2}$ (Fe^{2+})	724.94
		$2p_{3/2}$ (Fe^{3+})	723.28
		satellite	718.73
		$2p_{1/2}$ (Fe^{2+})	711.86
		$2p_{1/2}$ (Fe^{3+})	710.06
Cr	Cr 2p	$2p_{3/2}$ (Cr^{2+})	588.04
		$2p_{3/2}$ (Cr^{3+})	585.85
		$2p_{1/2}$ (Cr^{2+})	578.74
		$2p_{1/2}$ (Cr^{3+})	576.29
O	O 1s	O_{OH^-}	532.50
		$O_{vcan.}$	530.65
		O^{2-} (metal oxide)	529.47

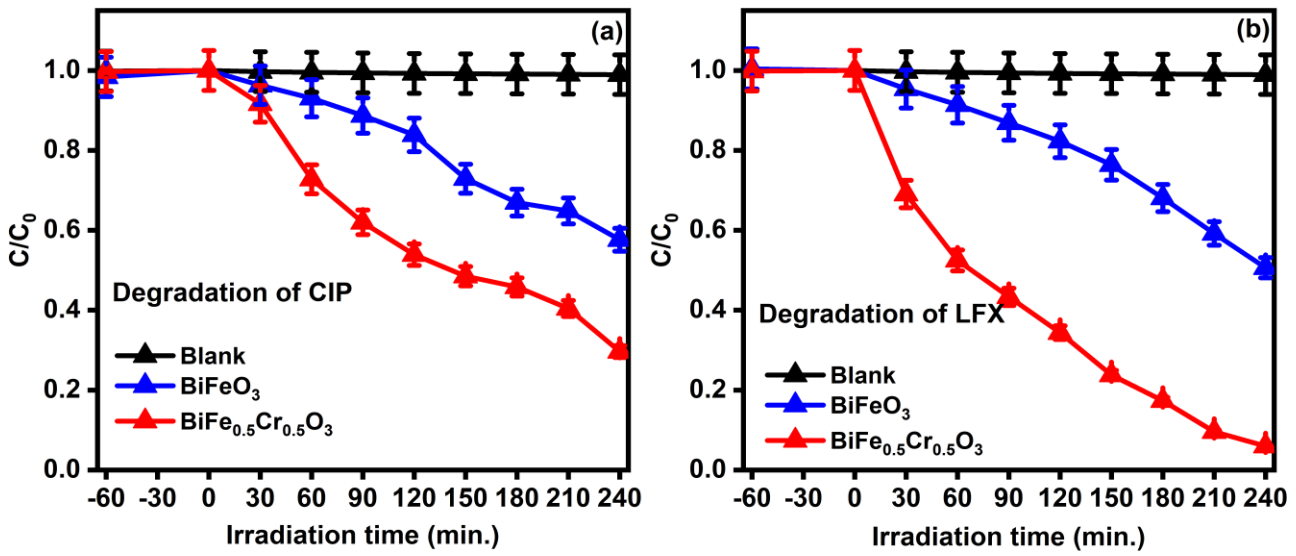

Fig. S5. *Comparative photocatalytic degradation of (a) CIP and (b) LFX in the presence of both the pristine $BiFeO_3$ and $BiFe_{0.5}Cr_{0.5}O_3$ photocatalyst.*

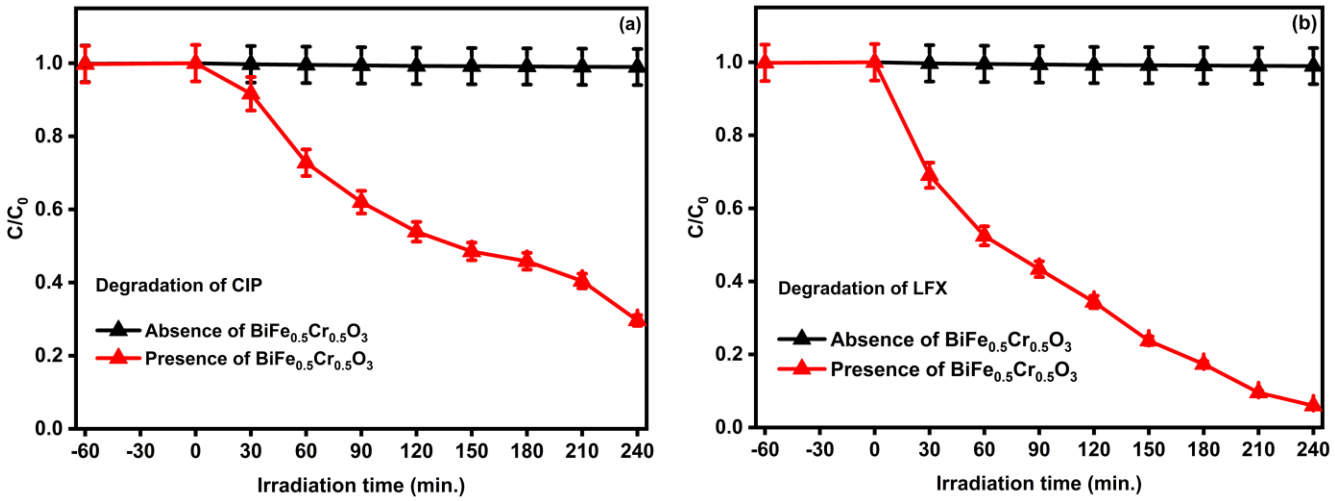

Fig. S6. *Photocatalytic degradation of (a) CIP and (b) LFX in the absence and presence of $BiFe_{0.5}Cr_{0.5}O_3$ photocatalyst.*

Apparent Quantum Yield (AQY) calculation

Step 1: Degraded pollutant molecule calculation

Detail	Unit	CIP ($BiFe_{0.5}Cr_{0.5}O_3$)	LFX ($BiFe_{0.5}Cr_{0.5}O_3$)
Pollutant solution	L	0.05	0.05
Pollutant concentration	g/L	0.01	0.01
Pollutant weight in solution	g	0.0005	0.0005
Molecular weight	g/mol	331.346	361.368
No. of moles in a solution	mol	1.51×10^{-6}	1.38×10^{-6}
No. of molecules in a mole	molecules/mol	6.02×10^{23}	6.02×10^{23}
Total no. of pollutant molecules	molecules	9.09×10^{17}	8.31×10^{17}
Degradation percentage	%	70.35	94
No. of degraded molecules	molecules	6.36×10^{17}	7.81×10^{17}

Step 2: Photon energy calculation

Wavelength of light λ = 440 nm = 440×10^{-9} m

Energy of one photon $E = \frac{hc}{\lambda} = \frac{6.6\times10^{-34}\times3\times10^{8}}{440 \times 10-9} = 4.50 \times 10^{-19}\ Joules$

The total energy of light falling per second per unit area is

$$E_{Total} = 100\ mW\ cm^{-2} = 100 \times 10^{-3} \times 10^{4} W\ m^{-2} = 1000\ W\ m^{-2}$$

Number of Photon = $\frac{E_{Total}}{\mathrm{E}} = \frac{1000}{4.50 \times 10^{-19}} = 2.22 \times 10^{21}$

Area of exposed solution = $\frac{2\pi rl}{2} = \pi rl$

Total number of Photon falling on the solution (Number of incident Photon) = Number of Photon × Area of exposed solution

Apparent Quantum Yield (AQY) = $\frac{Number\ of\ degraded\ molecule}{Number\ of\ incident\ photon} \times 100$

Irradiation time (min.)	Area of exposed solution (m^2)	Number of incident photon	Apparent Quantum Yield (%) in CIP ($BiFe_{0.5}Cr_{0.5}O_3$)	Apparent Quantum Yield (%) in LFX ($BiFe_{0.5}Cr_{0.5}O_3$)
240	0.001007	2.24×10^{18}	28.4	34.9

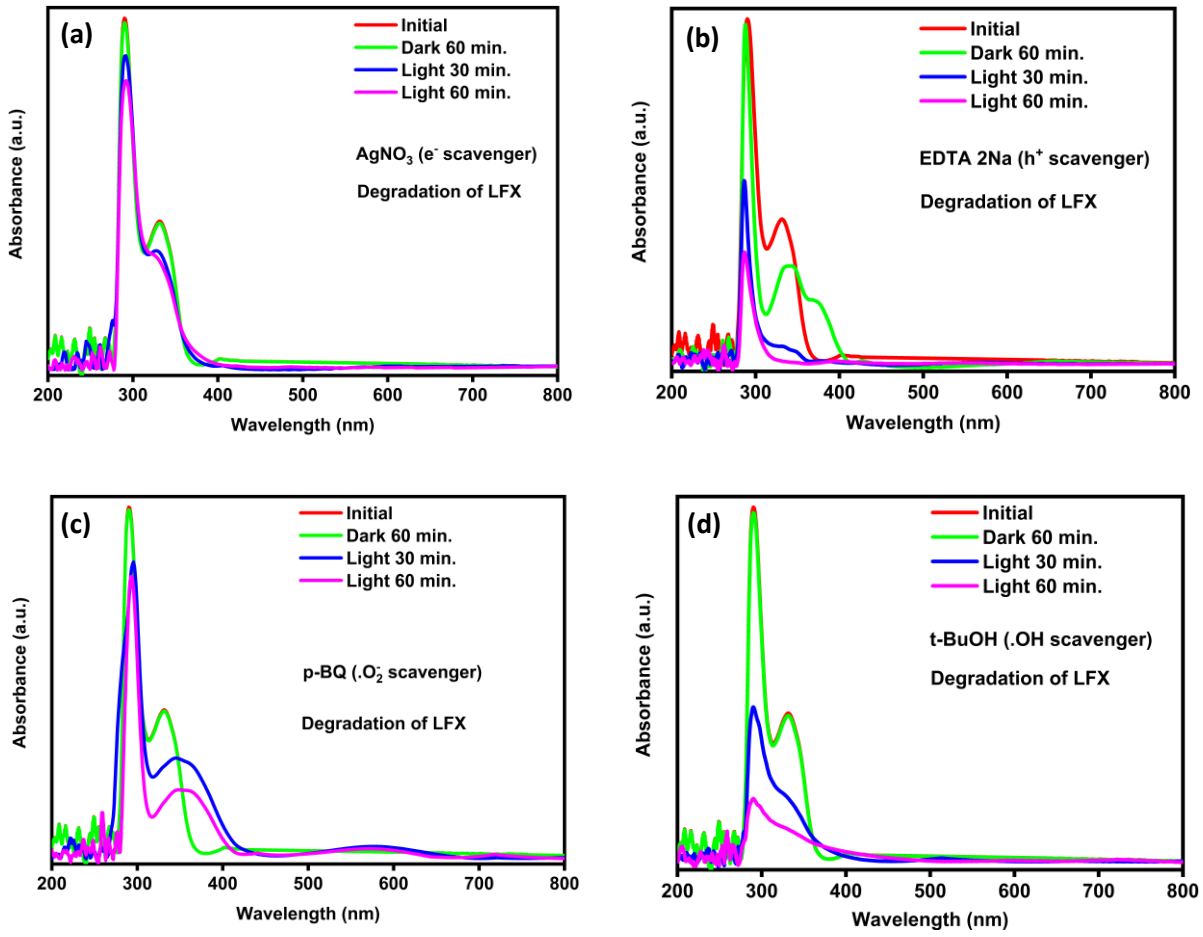

Fig. S7. *Photocatalytic degradation of LFX in the presence of $BiFe_{0.5}Cr_{0.5}O_3$ photocatalyst and (a) $AgNO_3$, (b) EDTA 2Na, (c) p-BQ and (d) t-BuOH trapping reagents.*

References:

1. T. V. Rozario, F. Sharmin, S. Shamim and M. Basith, *Ceram. Int.,* 2024, **50**, 3606–3617.
2. M. Tarek, F. Yasmeen and M. A. Basith, *J. Mater. Chem. A*, 2024, **12**, 25475–25490.
3. F. Yasmeen, M. Tarek and M. A. Basith, *ACS Appl. Mater. Interfaces*, 2024, **16**, 47535–47550.