Supporting Information

Engineering Oxygen-Vacancy-Rich S-Scheme $CeSnO_3/Bi_2S_3$ Perovskite-Based Heterojunction with Dynamic Ce^{3+}/Ce^{4+} Redox Recycling: Efficient Photoactivation of Peroxymonosulfate towards Lindane Degradation, Antimicrobial Activity and Sustainable H_2 Production

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Text S1

2.6. Photocatalytic degradation of LN under simulated solar irradiations in aqueous media

SPME extraction for LN

Solid phase micro-extraction (SPME) technique was used to collect the sample (LN) from aqueous media. Lindane was extracted by exposing the SPME fiber in glass vials for 1 min, followed by thermal desorption in the GC inlet for 1. After each run, the fiber was rinsed with Milli-Q water using the dip-injection method to eliminate residual contaminants [1].

Quantitative determination of LN using GC-μECD

Gas chromatography coupled with a micro-cell electron capture detector (GC-μECD) was employed for the detection and quantification of lindane in aqueous samples. This analytical technique is highly sensitive toward halogenated organic compounds, enabling trace-level analysis in environmental and biological matrices. GC-μECD was selected due to its superior selectivity and sensitivity toward organochlorine pesticides compared to other conventional detectors, making it particularly suitable for lindane analysis [2]. The quantification of lindane was carried out using an Agilent 6890N GC system equipped with a μECD operated in splitless mode. Separation was achieved using an HP-5 capillary column (30 m × 0.25 mm I.D., 0.25 μm film thickness). The oven temperature program was set as follows: initial temperature of 50 °C (held for 2 min), ramped to 150 °C at 10 °C min^{-1} (held for 3 min), and further increased to 250 °C at 20 °C min^{-1} (held for 5 min). The injector and detector temperatures were maintained at 220 °C and 350 °C, respectively. High-purity nitrogen was used as the carrier gas at a flow rate of 2.7 mL min^{-1}.

Text S2

2.7. Assessment of acute and chronic toxicity

To evaluate the ecotoxicological impact of the photocatalytic degradation process, the Ecological Structure–Activity Relationship (ECOSAR) program, which is based on structure–activity

relationships (SARs), was employed. This assessment aimed to determine whether the proposed photocatalytic treatment of lindane (LN) qualifies as an environmentally benign and safe approach. The ecotoxicity of the parent contaminants and their respective degradation products (DPs) was evaluated by predicting both acute and chronic toxicities toward representative aquatic organisms including green algae, Daphnia and fish. ECOSAR is particularly applicable in this context, because both lindane (LN) and Its DPs possess relatively low molecular weights (generally <1000 g mol^{-1}), which fall within the operational domain of the model. Key toxicological endpoints, including the chronic value (ChV), half maximal effective concentration (EC_{50}), and lethal concentration (LC_{50}), were used to assess the potential toxicity of these compounds. Specifically, EC_{50} refers to the concentration of a compound that inhibits 50% of green algae growth after 96 hrs of exposure, while LC_{50} denotes the concentration that leads to 50% mortality in Daphnia and fish following 48 and 96 hrs of exposure, respectively. These parameters collectively provide insight into the potential ecological risks associated with the degradation products formed during the photocatalytic treatment process [3, 4].

Text S3

2.8. Assessment of antimicrobial properties

Using the agar well diffusion method under visible light irradiation, the antibacterial activity of the as-synthesized $CeSnO_3$, Bi_2S_3 and $CeSnO_3/Bi_2S_3$) was assessed against the Gram-negative bacterium Escherichia coli (*E.coli*) and the fungus Candida albicans (*C. albicans*).

Microbial Strains and Culture Preparation

Nutrient agar (NA) and Sabouraud Dextrose Agar (SDA) were used to obtain and maintain pure cultures of *E. coli* and *C. albicans*, respectively. Both strains were cultivated for the duration of the experiment at 37°C and 30°C, respectively, in nutritional broth for *E. coli* and Sabouraud dextrose broth for *C. albicans*. The turbidity of the microbiological suspensions was

brought down to 0.5 McFarland standard, which is roughly 1.5×10^8 CFU/mL for bacteria and 10^6 CFU/mL for yeast.

Preparation of Agar Plates and Inoculation

Molten nutritional agar (for *E. coli*) and SDA (for *C. albicans*) were added to sterile Petri plates, which were then left to solidify. To construct a confluent microbial lawn, 100 µL of the prepared microbial solution was evenly applied to the agar surface using a sterile cotton swab after it had solidified. The plates were left undisturbed for 10–15 min to allow absorption.

Well Formation and Sample Loading

A sterile cork borer was used to punch wells into the agar that were 6 mm in diameter. To assure homogeneity, the synthesized $CeSnO_3$, Bi_2S_3 CB30 samples were ultrasonically dissolved in sterile distilled water at a concentration of 5 mg/mL for ten min. Each dispersion was then gently pipetted into its corresponding well, containing 100 µL of dispersion.

Visible Light Irradiation

Following sample loading, a white LED lamp with a wavelength range of 400–700 nm was placed at a fixed distance of 15 cm to expose the infected plates to visible light. At room temperature, the irradiation was carried out for 30 min. Care was taken to ensure uniform exposure of all plates.

Incubation and Measurement

The plates were incubated for 24 hrs at 37°C for E. coli and 24-48 hrs at 30°C for Candida albicans after light treatment. Following incubation, a digital caliper was used to measure the diameter of the zones of inhibition surrounding each well in mm.

Table S1 Chemical composition of TW, SW and IW

Water Type	HCO_3^- (mg L^{-1})	CO_3^{2-} (mg L^{-1})	Ca^{2+} (mg L^{-1})	Fe^{2+} (mg L^{-1})	NO_2^- (mg L^{-1})	SO_4^{2-} (mg L^{-1})	Cl^- (mg L^{-1})	Mg^{2+} (mg L^{-1})	HA (mg L^{-1})
TW	0.545	0.677	__	0.236	0.435	0.944	0.165	__	__
SW	1.173	1.073	__	1.049	1.087	1.188	1.101	__	0.226
IW	16.83	__	2.50	0.22	Nil	26.43	12.95	3.84	__

Table S2 Comparison of catalytic systems reported in literature for lindane degradation under different experimental conditions.

Catalyst system	Oxidant/Process	$[Lindane]_0$	$[Catalyst]_0$	Reaction Time	% Degradation	Reference
S-TiO_2/PMS	PMS (0.2 mM), visible light	1.0 µM	0.23 g L^{-1}	6 h	99.9%	[5]
Solar/TiO_2	Photocatalysis (no oxidant)	2.6 µg L^{-1}	0.5 g L^{-1}	10 h	25.77 %	[1]
UV/PS	Sulfate radical oxidation	3.43 µM	100 µM	2 h	93.2%	[6]
SSLA-TiO_2/PS	Photocatalysis with persulfate	~1 mg L^{-1}	0.5 g L^{-1}	6 h	~89 %	[7]
N-doped TiO_2	UV/visible photocatalysis	0.1 mg L^{-1}	1 g L^{-1}	7 h	~95 %	[8]
Persulfate/ Ferrioxalate/ Solar process	Simulated solar light	5 mg L^{-1}	0.12 mM	2 h	~95 %	[9]
$CeSnO_3$/Bi_2S_3 (This work)	**PMS (1.5 mM), visible light**	**600 µg L^{-1}**	**15 mg**	**100 min**	**93.21%**	**This work**

Table S3 Eco-toxicity assessment of LN, MV and their DPs towards aquatic organisms (mg L^{-1} [a]).

Compound/DPs	Acute toxicity			Chronic toxicity		
	LC_{50}		EC_{50}	ChV		
	Fish (Duration 96 h)	Daphnia (Duration 48 h)	Green Algae (Duration 96 h)	Fish	Daphnia	Green Algae
LN	2.24	1.57	2.76	0.28	0.27	1.15
DP1	0.52	0.48	1.31	0.05	0.04	0.76
DP2	1.26	1.14	2.68	0.17	0.06	1.25
DP3	0.08	0.06	0.211	0.012	0.017	0.12
DP4	8.52	5.45	6.62	0.95	0.73	2.26
DP5	2.72	2.27	0.25	0.31	0.32	0.75
DP6	27.6	325	5.87	17.8	129	0.67
DP7	3.16×10^3	3.80×10^3	1.53×10^3	2.12×10^3	388	221
DP8	718	282	53.3	63.1	24.3	215
DP9	4.85×10^4	2.24×10^3	711	372	123	118

[a]Acute toxicities based on the European Union criteria (described in Annex VI of Directive 67/548/EEC); Not harmful, Harmful, Toxic, and very toxic. While chronic toxicities evaluation based on the Chinese hazard evaluation criteria for new chemical substances (HJ/T154–2004); Not harmful, Harmful, Toxic, and very toxic.

Table S4 Antimicrobial activities analysis $CeSnO_3$, Bi_2S_3 and CB30 against *E. coli* and *C. albicans* using well diffusion method.

Sample	***E. coli* ZOI (mm)**	**Average ZOI (mm)**	***C. albicans* ZOI (mm)**	**Average ZOI (mm)**
$CeSnO_3$	18 & 15	16.5	16 & 19	17.5
Bi_2S_3	17 & 20	18.5	16 & 21	18.5
CB30	20 & 23	21.5	19 & 21	20

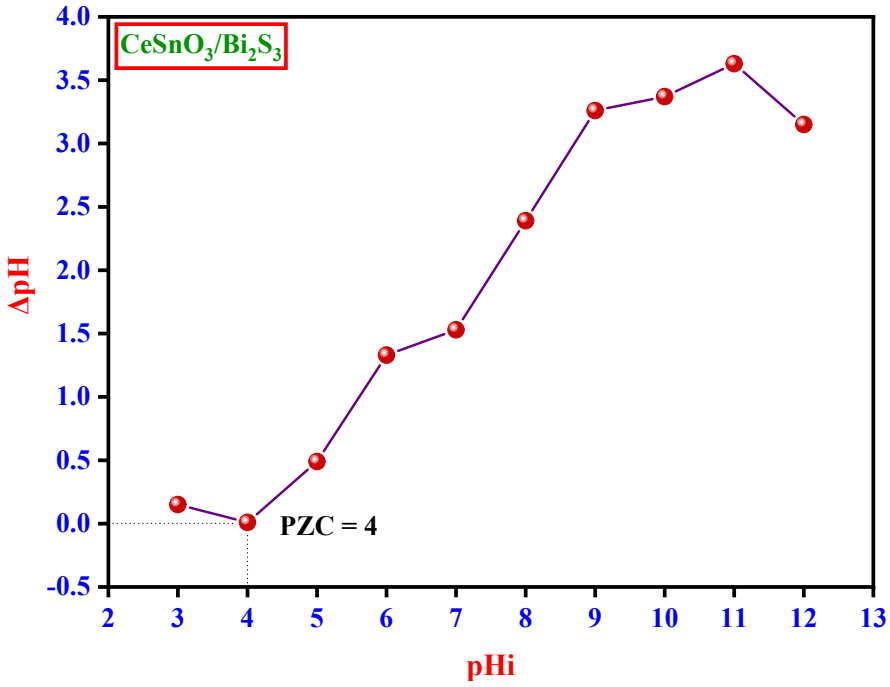

Fig. S1. PZC analysis of as-synthesized CB30 using salt addition method. Experimental conditions: [CB30] = 15 mg; [$NaNO_3$] = 0.1 M; [HNO_3] = 0.1 M; [NaOH] = 0.1 M.

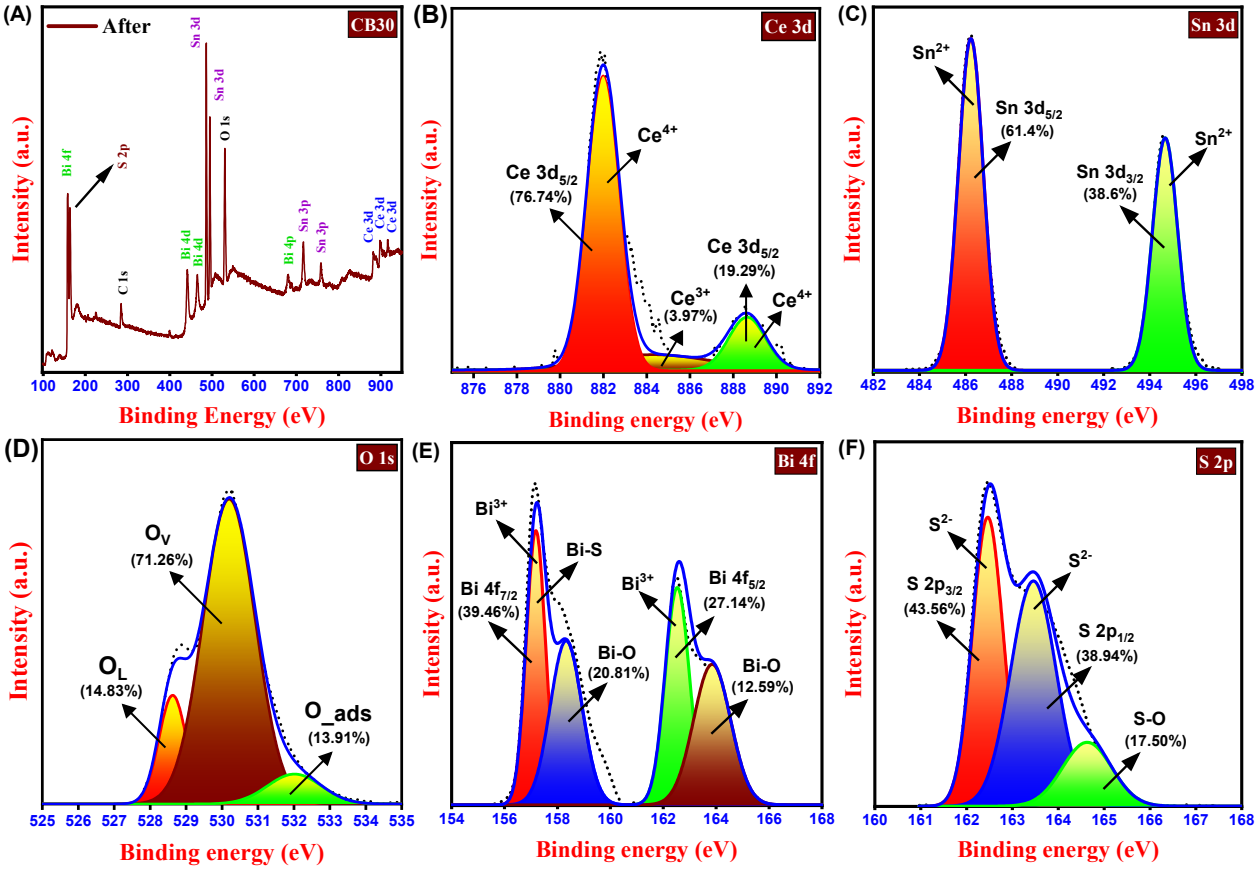

Fig. S2. XPS analysis of as-synthesized CB30 after illumination: Full length spectra (A), high resolution spectra of Ce (B), Sn (C), O (D), Bi (E) and S (F).

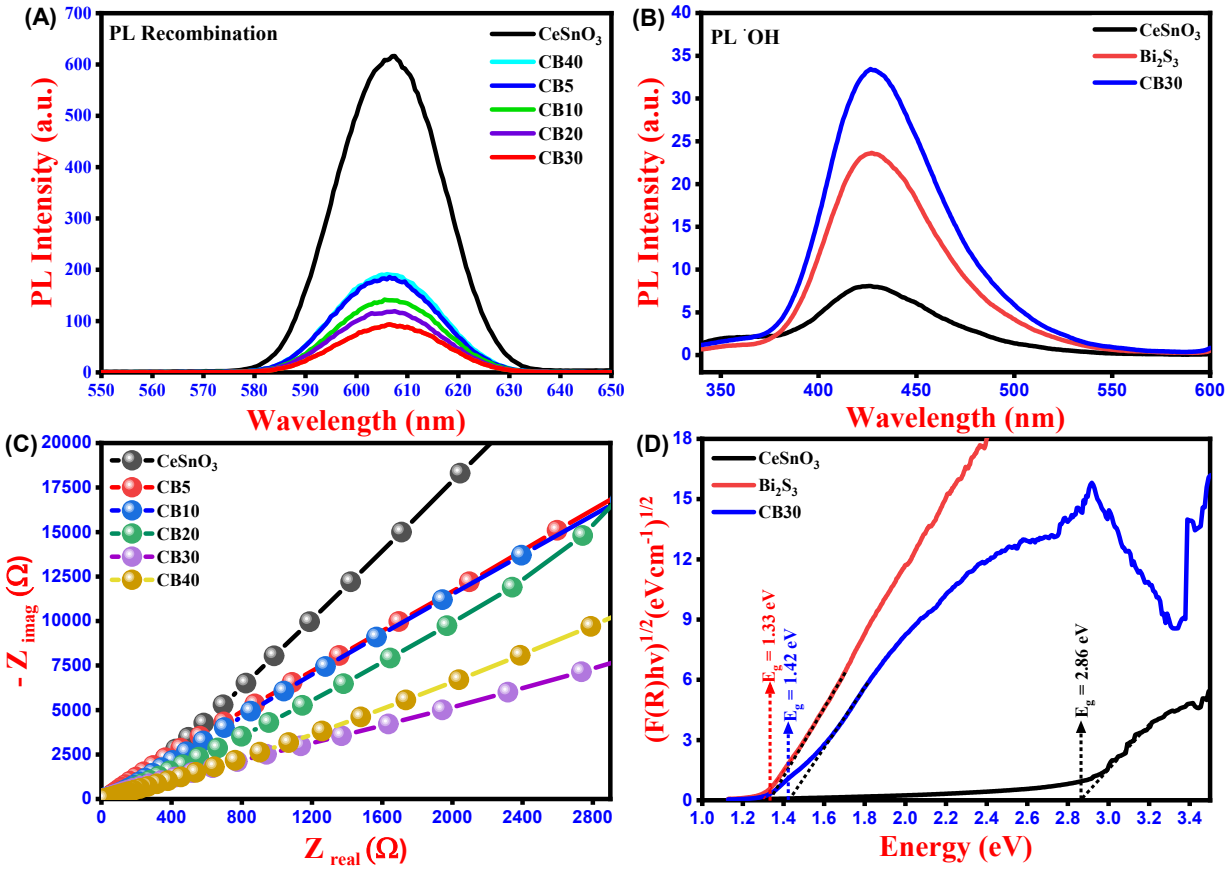

Fig. S3. PL recombination (A), PL for ˙OH formation (B) EIS Nyquist plots (C) and UV–vis DRS (D) of as-synthesized materials.

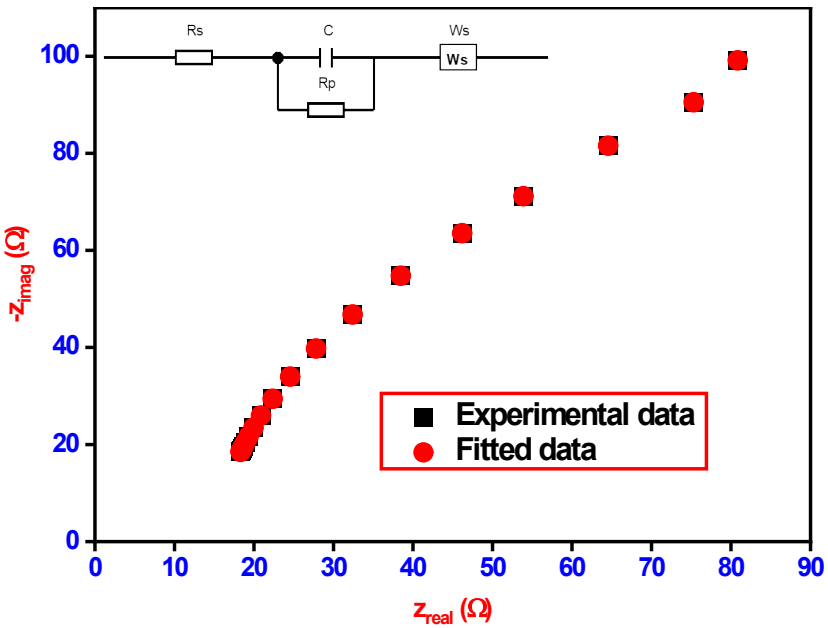

Fig. S4. Nyquist impedance plot of CB30 with equivalent circuit inset (Rs–(C‖Rp)–Ws model), showing experimental EIS data and the corresponding fitted response.

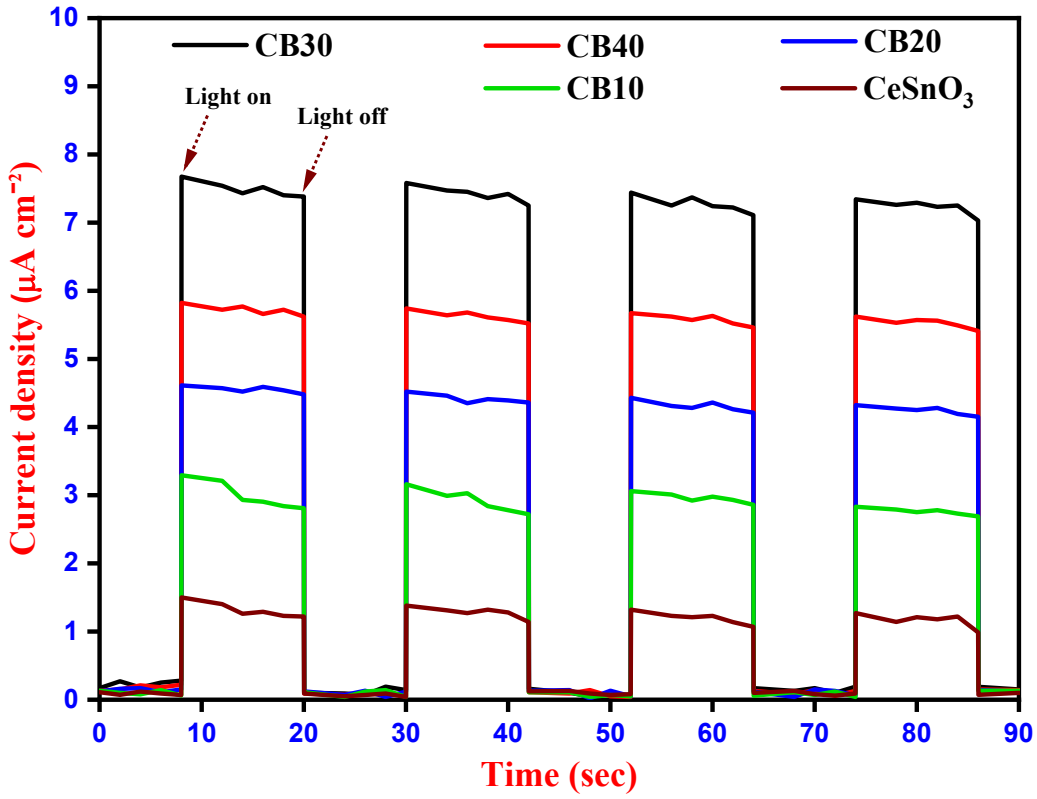

Fig. S5 Photocurrent response of as-synthesized $CeSnO_3$, CB10, CB20, CB30 and CB40 heterojunctions.

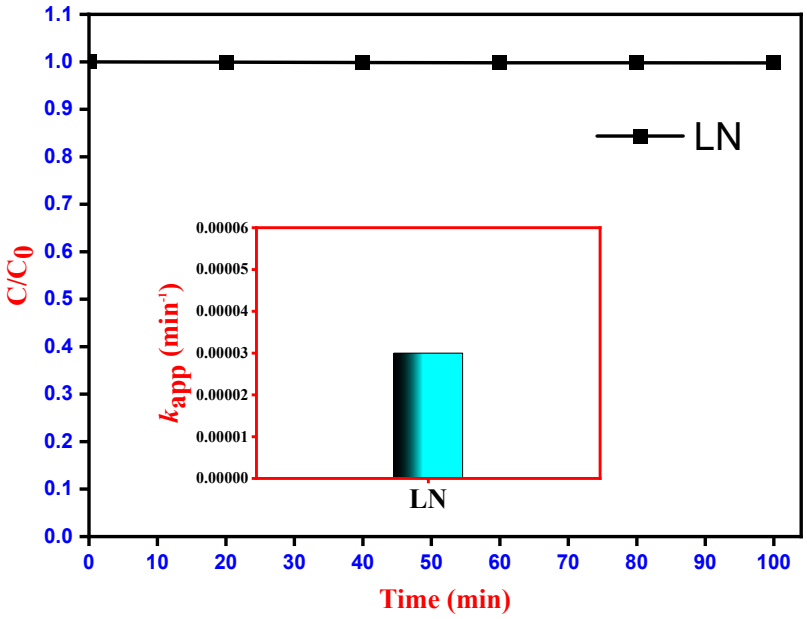

Fig. S6. Photolysis of LN under simulated solar light illumination for 100 min in aqueous media.

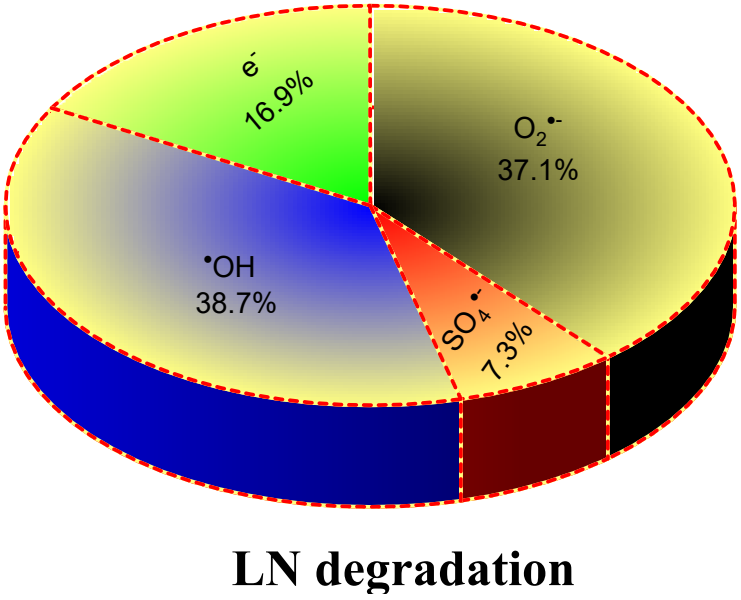

Fig. S7. Percent contribution reactive species in the photocatalytic degradation of LN**.**

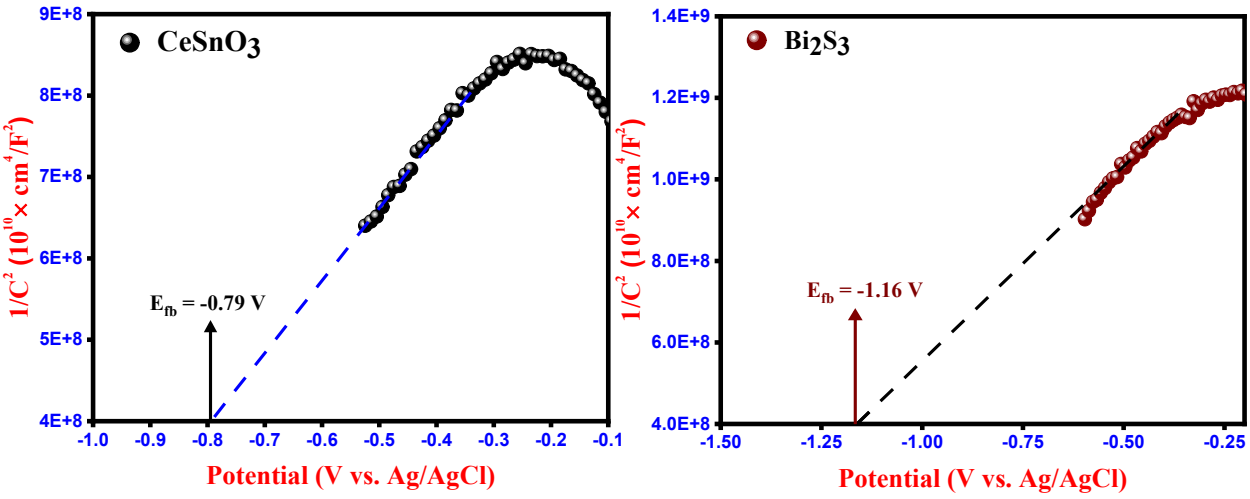

Fig. S8. Mott-Schottky plots of $CeSnO_3$ (A) and Bi_2S_3 (B).

References

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