SUPPLEMENTARY INFORMATION

Highly efficient CuO@ZnHCC heterostructure enabling rapid sunlight-driven detoxification of persistent organic dyes

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Text S1: Preparation of *M. koenigii* leaf extract

The leaves of the *Murraya koenigii* (curry leaves) were gathered from Malaviya National Institute of Technology (MNIT), Jaipur, in order to prepare the leaf extract for the environmentally friendly production of nanoparticles. To obtain the freshly made extract, the 5 g of gathered leaves were properly cleaned with deionized water, allowed to dry overnight, and then ground in a mortar and pestle before being filtered. The PE solution was kept in storage at 4°C for use in synthesis. Phytochemicals that function as natural reducing and stabilizing agents, including mahanimbine, koenimbine, flavonoids, phenolic compounds, alkaloids, tannins, and terpenoids, are abundant in *M. koenigii* leaves. By stabilizing the metal ions by capping their surfaces, these biomolecules help reduce them to nanoparticles and stop them from aggregating. Alkaloids, saponins, and terpenoids aid in controlling particle size and improving the colloidal stability of the produced nanoparticles, while the extract's polyphenols and flavonoids act as electron donors for the reduction process.

Text S2: Instrumentation

The PAN analytical X-PRT PRO instrument was used to obtain powder X-ray diffraction (PXRD) spectra with a Cu Kα radiation with λ=1.5406 Å. Using an Image Analyzer instrument scanning (SEM, Hitachi S4800) and a Model JSM6100 (Jeol), Field-Emission Scanning Electron Microscopy (FE-SEM) was used to examine the morphology of the photocatalysts. Omicron nanotechnology (ESCA+) X-ray photoelectron spectroscopy (XPS) measurements were made using Oxford instrumentation. To determine the bonding in the nanocomposite, Fourier transform infrared spectra (FT-IR) were acquired using a Perkin Elmer spectrophotometer version 10.4.00 in the 400–4000 cm^{-1} range. Malvern Zetasizer (Zetasizer Ver. 7.11) was used to measure the zeta potential in order to assess the stability of the photocatalysts. The UV Spectrophotometer (Agilent Pro) was used to measure the absorbance

of the samples. Additionally, LABWAN-PH-61WW devices were utilized to prepare pH solutions for total organic carbon (TOC) analysis using the TOC-L analyzer Shimazu, and the CPA-225D Sartius Analytical balance was employed for weighing purposes.

Text S3: Statistical analysis

In the kinetics investigation, Origin Pro was utilized to create graphs, and statistical analyses of the experimental data for the elimination of specific pollutants (MB and TOOO) by nanocomposite were empirically represented from an asymptotic analysis. The standard deviation was calculated using the "Microsoft Excel" program, and the results were well accepted in triplicate. By comparing the outcomes using the beta coefficient (R^2) and probability values (p-values), the experimental data's relevance was demonstrated. A number of models, including the Freundlich, Temkin, Dubinin-Radushkevich (DRK), and Langmuir isotherms, were employed to analyze the adsorption data. Plots of adsorption isotherms at various concentrations have been made using a straight line (Y= mX + c) linear curve.

Specifications of the D-R, Temkin, Sip, Freundlich, and Langmuir isotherms utilized in this investigation

Ce/Xe v/s Ce of the solute was used to compute adsorption data using Langmuir adsorption isotherms. Which were determined by using the equation to match the adsorption data:

$$\frac{C_e}{X_e} = \frac{1}{k_L X_m} + \frac{C_e}{X_m}$$

or

$$\frac{1}{X_e} = \frac{1}{C_e}\left(\frac{1}{k_L X_m}\right) + \frac{1}{X_m}$$

X_e was calculated through the equation:

$$X_e = \frac{(Ci - Ce) \times Volofsolution(mL) \times Molecularweightofadsorbent}{Amountofcatalyst\ (mg)}$$

Freundlich Isotherm:

The solute's Xe vs. Ce graph was often a straight line. $Xe = Kf + Ce1/n$ and linear form is

$$\log Xe = \log Kf + \frac{1}{n} logCe$$

where Xe is the quantity of dye adsorbed per gram weight of adsorbent, K_f is the Freundlich adsorption constant (mg/g), n is the adsorption intensity, and Ce is the dye solution's equilibrium concentration.

Temkin Isotherm:

$$Xe = \frac{RT}{b} \ln A + \frac{RT}{b} \ln Ce$$

where A (slope) = Temkin isotherm equilibrium binding constant (L/g); b (intercept) = Temkin isotherm constant; R = universal gas constant (8.314 $J \cdot mol^{-1} \cdot K^{-1}$) and B = RT/b constant connected to heat of sorption (J/mol) derived from the Temkin plot (Xe v/s ln Ce); T = 298, 308, and 318 K temperatures.

Dubinin-Radushkevich (D-R) isotherm:

$$\ln Xe = \ln Xm - \beta\varepsilon 2$$

$$\varepsilon = RTln\left(1 + \frac{1}{Ce}\right)$$

where ε is the Polanyi potential, β (mol^2/J^2) is an activity coefficient constant associated with sorption energy, and Xm is the maximum adsorption capacity (mg/g) determined from the intercept. Plotting D-R between ln Xe Vs ε^2 was done.

Sips Isotherm:

Between 1/Xe $\times 10^{-2}$ (g/mg) and (1/Ce) $\times 10^{-8}$ L/mg, it is plotted; the Sips equilibrium constant and maximum adsorption capacity values are (1/mg) and (mg/g), respectively, derived from the plot's slope and intercept. The dimensionless heterogeneity factor "n," which is used to characterize the Sips isotherm equation, can also be used to quantify the heterogeneity of the system when it falls between 0 and 1.

$$\frac{1}{X_e} = \frac{1}{XmKs}\left(\frac{1}{Ce}\right)1/n + \frac{1}{X_m}$$

Tables and Figures

Table 1S. Details of angle, Fwhm values, interplanar spacing and hkl values of CuO, ZnHCC, and CuO@ZnHCC nanocomposite respectively.

a. CuO

Angle (2θ)	Fwhm values	d-spacing (Å)	hkl values
32.7262	0.1338	2.73650	(111)
34.7304	0.2676	2.58304	(111)
35.7341	0.2509	2.51276	(200)
38.9375	0.2175	2.31309	(020)
41.9981	0.2007	2.15134	(210)
46.4712	0.2676	1.95415	(211)

48.9042	0.1338	1.86247	(211)
53.6323	0.2676	1.70890	(220)
58.4689	0.2676	1.57855	(310)
61.7447	0.3011	1.50243	(311)
65.9468	0.2342	1.41651	(222)
66.4323	0.1338	1.40734	(222)
68.2617	0.1004	1.37401	(320)
72.5639	0.3346	1.30279	(321)
75.3825	0.1338	1.26092	(400)

b. ZnHCC.

Angle (2θ)	**Fwhm values**	**d-spacing (Å)**	**hkl values**
19.1444	0.5353	4.63610	(111)
31.9668	0.3011	2.79976	(220)
34.5894	0.4015	2.59325	(310)
36.4055	0.3346	2.46794	(311)
39.1564	0.4684	2.30066	(320)
47.7320	0.5353	1.90543	(331)
56.6902	0.2676	1.62377	(431)

62.9868	0.6691	1.47576	(440)
68.1430	0.6691	1.37612	(532)

c. CuO@ZnHCC.

Angle (2θ)	Fwhm values	d-spacing (Å)	hkl values
31.9365	0.2007	2.80235	(111)
32.7183	0.2007	2.73714	(111)
34.6580	0.2342	2.58827	(200)
35.7285	0.2676	2.51313	(002)
36.4610	0.1673	2.46431	(020)
38.9109	0.2676	2.31461	(200)
41.9876	0.2676	2.15185	(210)
47.7206	0.5353	1.90586	(211)
49.0151	0.2676	1.85852	(211)
53.7125	0.4015	1.70654	(220)
56.7396	0.3346	1.62248	(300)
58.3494	0.4015	1.58149	(310)
61.7696	0.4015	1.50188	(311)

63.0795	0.4015	1.47381	(222)
66.4897	0.4015	1.40626	(222)
68.2095	0.3346	1.37494	(321)
72.5558	0.4015	1.30291	(400)
75.2956	0.5353	1.26216	(410)

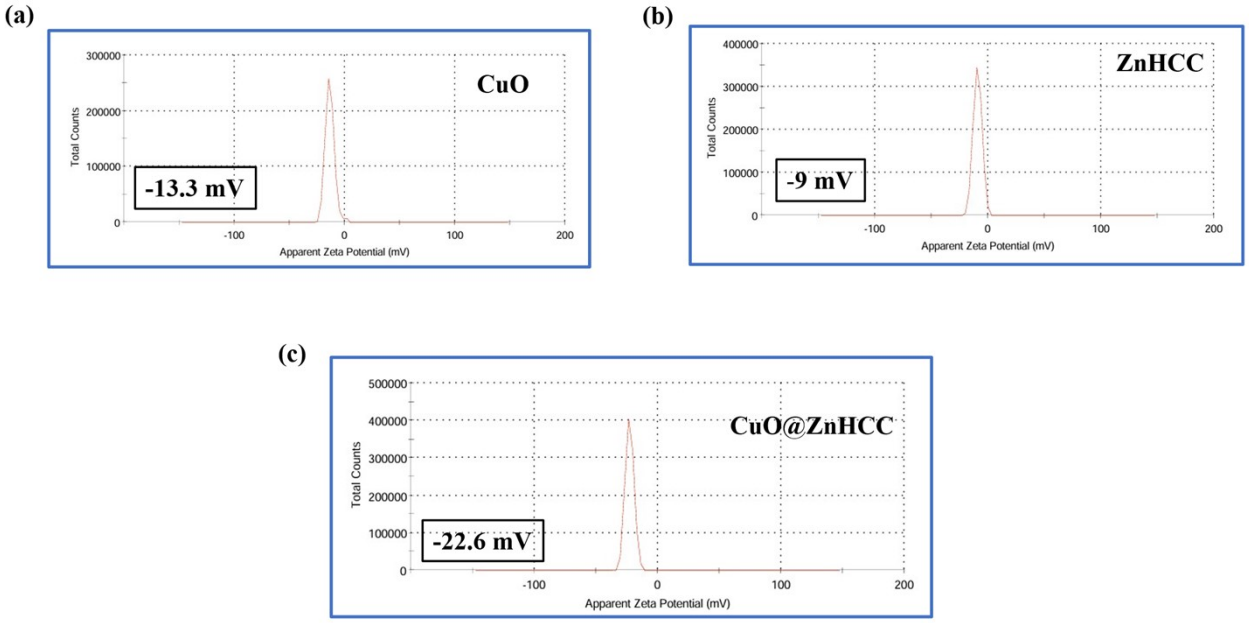


Figure 1S. Zeta potential of (a) CuO (b) ZnHCC and (c) CuO@ZnHCC nanocomposite respectively.

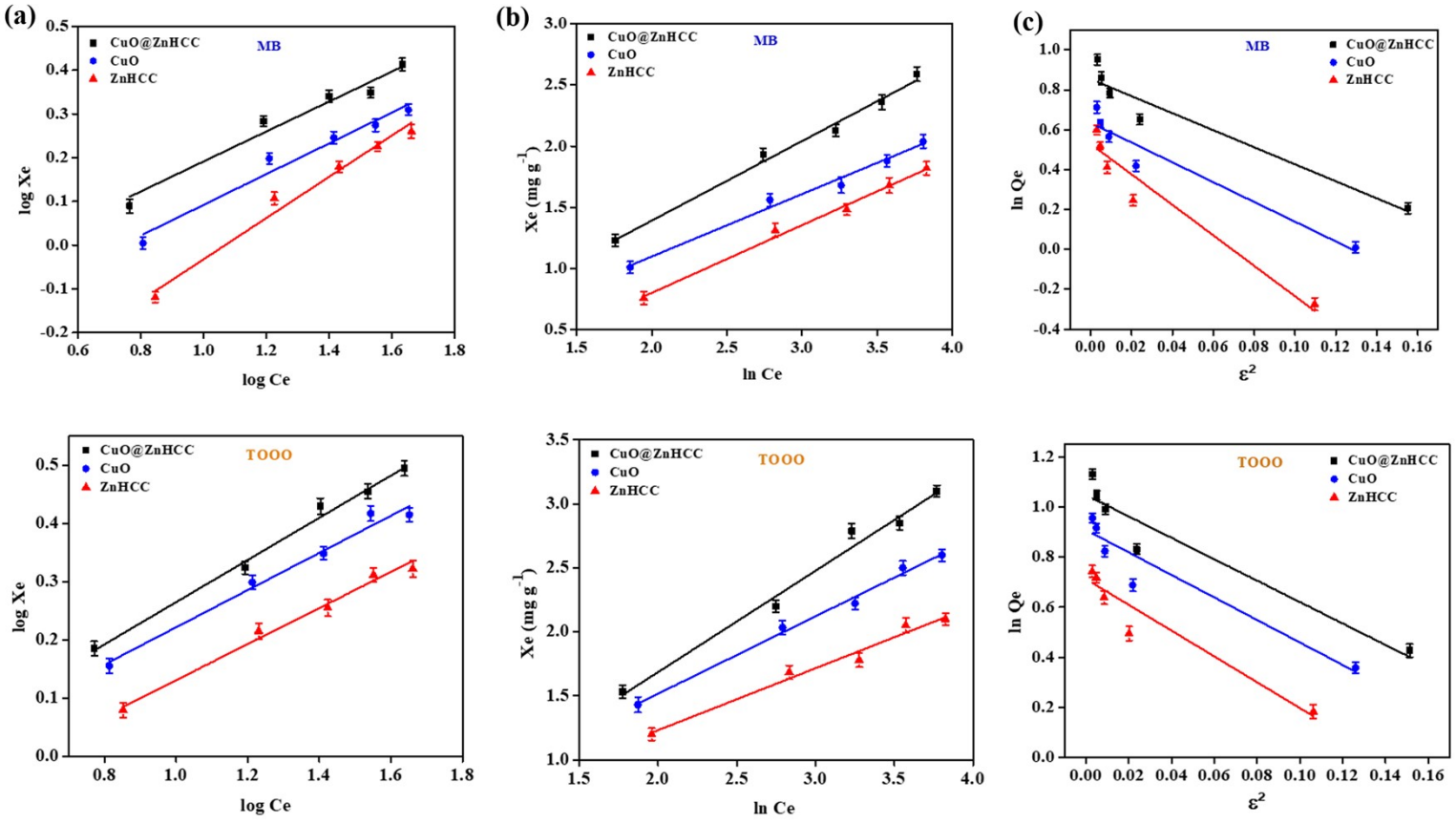


Figure 2S. (a) Freundlich (b) Temkin and (c) D-R isotherms for MB and TOOO adsorption.

Note: Triplicate experiments (n=3) were evaluated for estimation of error bar.

Table 2S. Comparison of different isotherms on the basis of R^2 and p values for MB and TOOO adsorption.

	Langmuir				**Temkin**			
	MB		**TOOO**		**MB**		**TOOO**	
Catalyst	**R^2**	**p**	**R^2**	**p**	**R^2**	**p**	**R^2**	**p**
CuO@ZnHCC	0.99	0.003	0.99458	0.003	0.9904	0.47	0.98594	0.59
CuO	0.99819	0.0008	0.99662	0.003	0.98917	0.46	0.99171	0.05

ZnHCC	0.99884	0.0001	0.99784	0.001	0.99365	0.03	0.98233	0.11

	DRK				**Freundlich**			
	MB		**TOOO**		**MB**		**TOOO**	
Catalyst	**R^2**	**p**	**R^2**	**p**	**R^2**	**P**	**R^2**	**p**
CuO@ZnHCC	0.92392	0.0003	0.89829	0.0001	0.95703	0.07	0.99217	0.02
CuO	0.93412	0.0006	0.92172	0.0002	0.96736	0.01	0.98107	0.06
ZnHCC	0.92582	0.0017	0.92784	0.0002	0.98466	0.001	0.98783	0.006

Table 3S. Reduced chi square and Adj. R square values of kinetics model for MB and TOOO pollutants.

	Langmuir						**Temkin**					
	MB			**TOOO**			**MB**			**TOOO**		
Catalyst	**Adj. R^2**	**Red. Chi^2**	**DOF**	**Adj. R^2**	**Red. Chi^2**	**DOF**	**Adj. R^2**	**Red. Chi^2**	**DOF**	**Adj. R^2**	**Red. Chi^2**	**DOF**
CuO@ZnHCC	0.99342	0.48049	3	0.99277	0.65462	3	0.98726	1.1927	3	0.98125	2.90417	3
CuO	0.99759	0.30332	3	0.99549	0.53106	3	0.98556	0.87002	3	0.98894	0.76803	3
ZnHCC	0.99845	0.19801	3	0.99712	0.51255	3	0.99153	0.51054	3	0.97664	1.23683	3

	DRK						Freundlich					
	MB			TOOO			MB			TOOO		
Catalyst	**Adj. R^2**	**Red. Chi^2**	**DOF**	**Adj. R^2**	**Red. Chi^2**	**DOF**	**Adj. R^2**	**Red. Chi^2**	**DOF**	**Adj. R^2**	**Red. Chi^2**	**DOF**
CuO@ZnHCC	0.89856	11.13433	3	0.86438	18.1138	3	0.9427	3.48012	3	0.98957	1.04306	3
CuO	0.91216	9.77696	3	0.89563	14.83234	3	0.9564	3.4414	3	0.97477	1.82559	3
ZnHCC	0.90109	14.2222	3	0.90379	7.57204	3	0.9795	2.97745	3	0.98377	0.95383	3

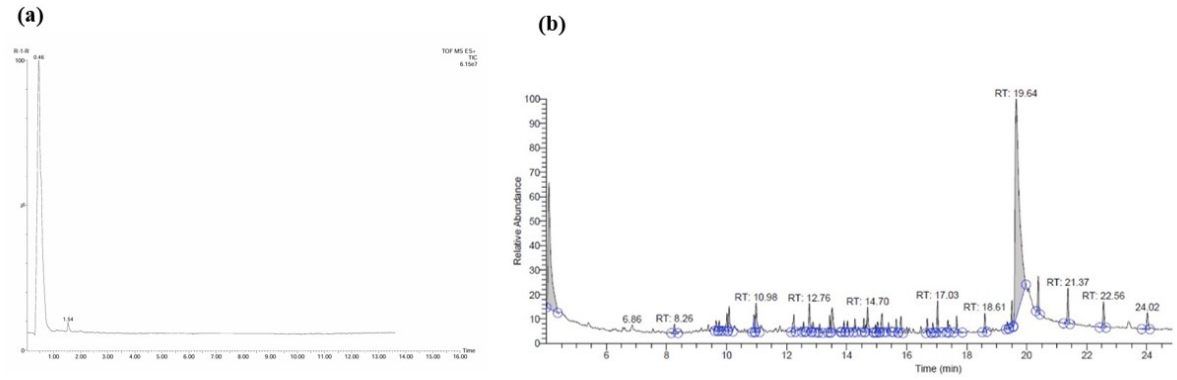
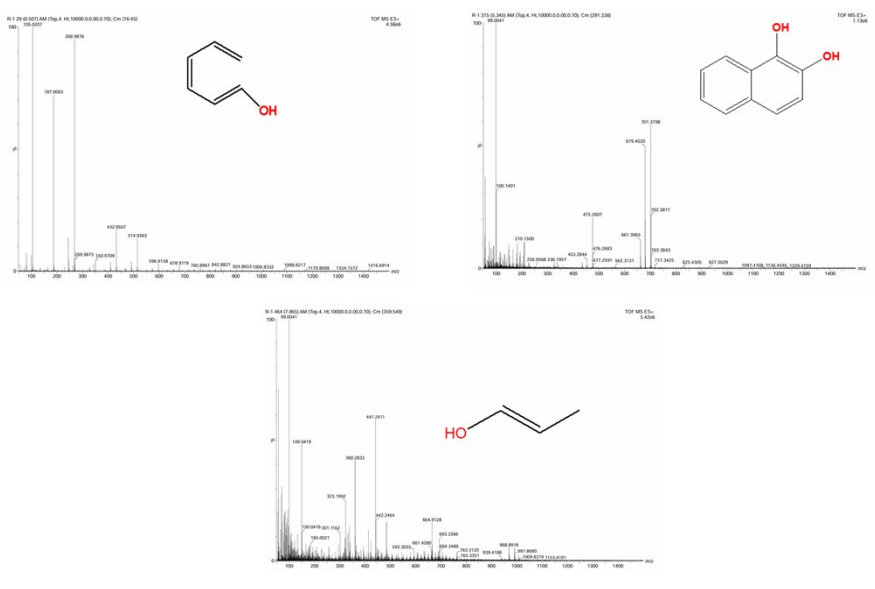
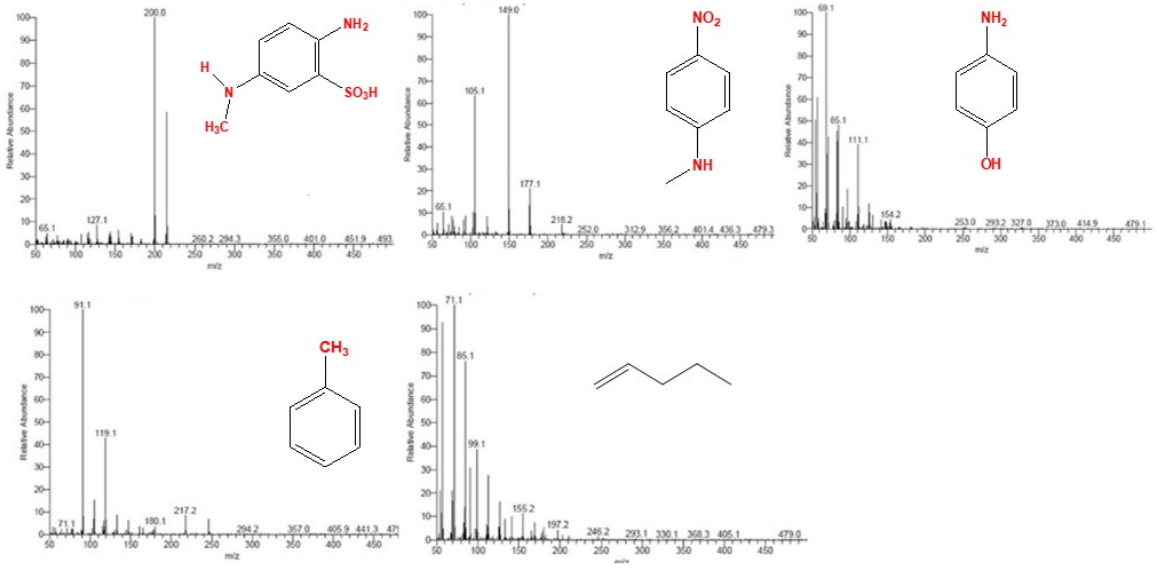


Figure 3S. Total Ion chromatogram (TIC) of degraded (a) TOOO and (b) MB

(a) TOOO



(b) MB



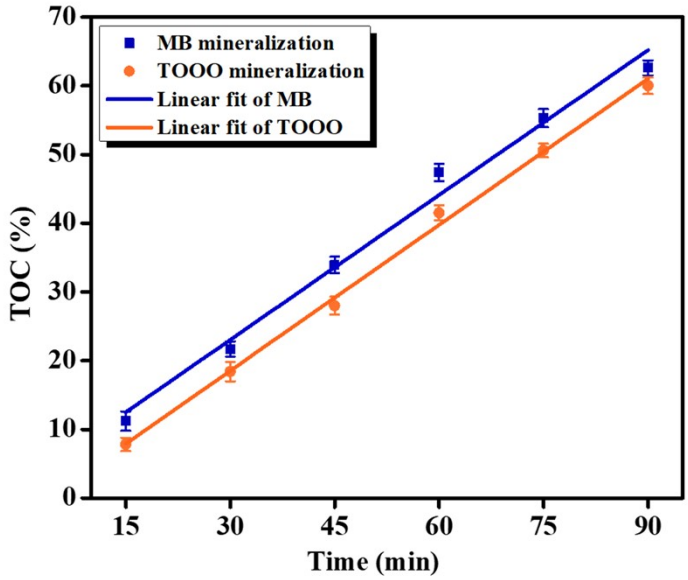


Figure 4S. Mass spectra of degraded (a) TOOO and (b) MB.

Figure 5S. TOC analysis and mineralization efficiency of targeted dyes (MB and TOOO) over the CuO@ZnHCC.

Text S4: Turn over frequency (TOF)

As is well known, a catalyst's TOF dictates its efficiency; the higher the TOF, the more effective the catalyst. The following formula can be used to determine the TOF value:

$$\frac{No\ of\ moles\ of\ reactant/No\ of\ grams\ of\ photocatalysts}{Time\ (min)} X\ yield$$

No of gram of photocatalyst: 0.1 g. (10 ppm)

Table 4S. TOF of CuO, ZnHCC and CuO@ZnHCC for MB and TOOO pollutants.

S.No.	**Photocatalyst**	**TOF (mol $min^{-1}g^{-1}$)**	
		MB	**TOOO**
1.	CuO@ZnHCC	1.07×10^{-3}	1.03×10^{-3}
2.	ZnHCC	8.26×10^{-4}	8.6×10^{-4}
3.	CuO	8.87×10^{-4}	8.01×10^{-4}