Supplementary information

Efficient and recyclable Nd³⁺-doped CoFe₂O₄ for boosted visible light-driven photocatalytic degradation of Rhodamine B dye

Loan T. T. Nguyen,¹ Hang T. T. Nguyen,² Lan T. H. Nguyen,¹ Anh T. T. Duong,¹ Hai Q.

Nguyen,¹ Viet T. M. Ngo,¹ Nhuong V. Vu,¹ Duyen Thi Cam Nguyen,^{3,4} Thuan Van Tran^{3,4,*}

Affiliation

¹ Faculty of Chemistry, Thai Nguyen University of Education, Thai Nguyen 240000, Vietnam.

² Faculty of Automotive and Power Machinery Engineering, Thai Nguyen University of Technology, Thai Nguyen 24000, Vietnam.

³ Institute of Applied Technology and Sustainable Development, Nguyen Tat Thanh University, 298-300A Nguyen Tat Thanh, District 4, Ho Chi Minh City 755414, Vietnam.

⁴ Faculty of Environmental and Food Engineering, Nguyen Tat Thanh University, 298-300A Nguyen Tat Thanh, District 4, Ho Chi Minh City 755414, Vietnam.

Correspondence

* To whom correspondence should be addressed: Thuan Van Tran (Email: <u>tranvt@ntt.edu.vn</u>, <u>ttran@gradcenter.cuny.edu</u>, <u>tranuv@gmail.com</u>), Tel: (+84)-028-3941-1211, Fax: (+84)-028-39-404-759.

Chemicals

Several chemicals, e.g., $Co(NO_3)_2 \cdot 4H_2O$ (98.0%), $Nd(NO_3)_3 \cdot 6H_2O$ (99.0%), $Fe(NO_3)_3 \cdot 9H_2O$ (98.0%), and urea $CO(NH_2)_2$ (99.0%) in this work were purchased from Merck, USA.

Characterization

XRD patterns were conducted on the D8 Advance diffractometer (Brucker, Madison, WI, USA) with the CuK α radiation ($\lambda = 1.5406$ Å) beams as excitation sources.

The particle morphology and size of the samples were recorded on SEM technique on a multi-purpose scanning electron microscope JSM-6510 (JEOL/EO, Tokyo, Japan) equipped with energy dispersive X-ray (EDX) spectroscopy.

The optical absorption characterization of the photocatalysts were determined using UV-Vis DRS on the Hitachi U-4100 spectrophotometer (Hitachi, Kyoto, Japan) in the wavelength range of 200–900 cm⁻¹.

The N₂ adsorption/desorption isotherms for surface area and pore distribution measurements were determined using Brunauer–Emmett–Teller (BET) and Barrett–Joyner–Halenda (BJH) methods, respectively and recorded on the Micromeritics TriStar 3000 V6.07 (Micromeritics Inc., Norcross, GA, USA).



Fig. S1. UV–Vis diffuse reflectance spectra with Tauc plots of $(\alpha h\nu)^2$ against photon energy (hv) of (a) CoFe₂O₄, (b) CoNd_{0.01}Fe_{1.99}O₄, (c) CoNd_{0.03}Fe_{1.97}O₄, and (d) CoNd_{0.05}Fe_{1.95}O₄ catalysts.



Fig. S2. Magnetic properties of (a) $CoFe_2O_4$, (b) $CoNd_{0.01}Fe_{1.99}O_4$, (c) $CoNd_{0.03}Fe_{1.97}O_4$, and (d) $CoNd_{0.05}Fe_{1.95}O_4$ catalysts.



Fig. S3. Energy-dispersive X-ray spectroscopy analysis and chemical composition of (a)

 $CoFe_2O_4$, (b) $CoNd_{0.05}Fe_{1.95}O_4$ catalysts.



Fig. S4. The XRD patterns for fresh and reused $CoNd_{0.05}Fe_{1.95}O_4$ catalysts.

Table S1. The angle value (20) at lattice plane (331), particle size (r), typical FTIR absorbance bands of Nd–O bonds for tetrahedral sites (v_1) and octahedral sites (v_2) of CoNd_xFe_{2-x}O₄ (x = 0, 0.01, 0.03, 0.05) catalysts.

No	Catalyst	20 (°)	r (nm)	v_1 (cm ⁻¹)	$v_2 (cm^{-1})$
1	CoFe ₂ O ₄	35.27	14.35	551.6	424.3
2	$CoNd_{0.01}Fe_{1.99}O_4$	35.35	19.05	582.5	474.5
3	CoNd 0.03Fe1.97O4	35.51	26.74	590.2	482.2
4	CoNd _{0.05} Fe _{1.95} O ₄	35.60	29.14	591.0	484.5

Table S2. Textual properties of $CoNd_xFe_{2-x}O_4$ (x = 0, 0.05) catalysts.

Surface property	$CoNd_{x}Fe_{2-x}O_{4} (x=0)$	$CoNd_xFe_{2-x}O_4 \ (x = 0.05)$
Specific surface area	$12.7 (m^2 g^{-1})$	$35.0 (m^2 g^{-1})$
Total pore volume	$0.099 (cm^3 g^{-1})$	$0.114 (cm^3 g^{-1})$
Average pore width	32.8 (nm)	12.6 (nm)

Table S3. Degradation efficiency (H, %), degradation kinetic rate (k_1 , min⁻¹), coefficient of determination (R^2) of removal of RhB dye using various CoNd_xFe_{2-x}O₄ (x = 0, 0.01, 0.03, 0.05) catalyst under visible light.

No	Catalyst	Н (%)	$k_1 \cdot 10^3 \text{ (min}^{-1}\text{)}$	R ²
1	H ₂ O ₂ only	12.9	0.7	0.99
2	Catalyst only	29.4	1.4	0.98
3	$H_2O_2 + CoFe_2O_4$	71.7	3.9	0.99
4	$H_2O_2 + CoNd_{0.01}Fe_{1.99}O_4$	75.9	4.1	0.99
5	$H_2O_2 + CoNd_{0.03}Fe_{1.97}O_4$	88.2	4.9	1.00
6	$H_2O_2 + CoNd_{0.05}Fe_{1.95}O_4$	94.7	5.3	0.96

Table S4. Degradation efficiency (H, %), degradation kinetic rate (k_1 , min⁻¹), coefficient of determination (R^2) under CoNd_{0.05}Fe_{1.95}O₄ catalyst with and without addition of scavengers (e.g., ascorbic acid, ethylenediaminetetraacetic acid (EDTA), and isopropyl alcohol).

ZnLa _{0.05} Fe _{1.95} O ₄	No scavenger	With ascorbic acid	With isopropyl	With EDTA
			alcohol	
Н (%)	93.7	61.6	52.1	49.8
$k_1 \cdot 10^3 (min^{-1})$	5.3	3.4	2.9	2.7
R ²	0.96	0.99	1.00	0.99

Note: $[RhB] = 10 \text{ mg } L^{-1}$, Duration = 0–180 min, $[H_2O_2] = 0.1 \text{ M}$, $[catalyst] = 0.75 \text{ g } L^{-1}$, V = 100 mL, $T = 25 \pm 1 \text{ °C}$, agitation speed: 200 rpm, and pH 7 under LED visible light source.