

Support Information

Bicomponent CuO/NiCo₂O₄ Nanocomposites for Dehydrogenation of Ammonia Borane and Tandem Hydrogenation of Halogenated Nitroaromatics

Xusheng Yang ^a, Ping Li^a, Jiahao Wu^a, Le Zhou^a, Bin Xu^{a**}, Xiaobin Zhang^b,

Xiaoqiang Liu^a, Pingchuan Pan^b, Weidong Jiang^{a*}

[†] School of Chemistry and Environmental Engineering, Sichuan University of Science & Engineering, Sichuan Zigong 643000, P. R. China;

[‡] Radiation Chemistry Department, Sichuan Institute of Atomic Energy, Sichuan Chengdu 610101, P. R. China.

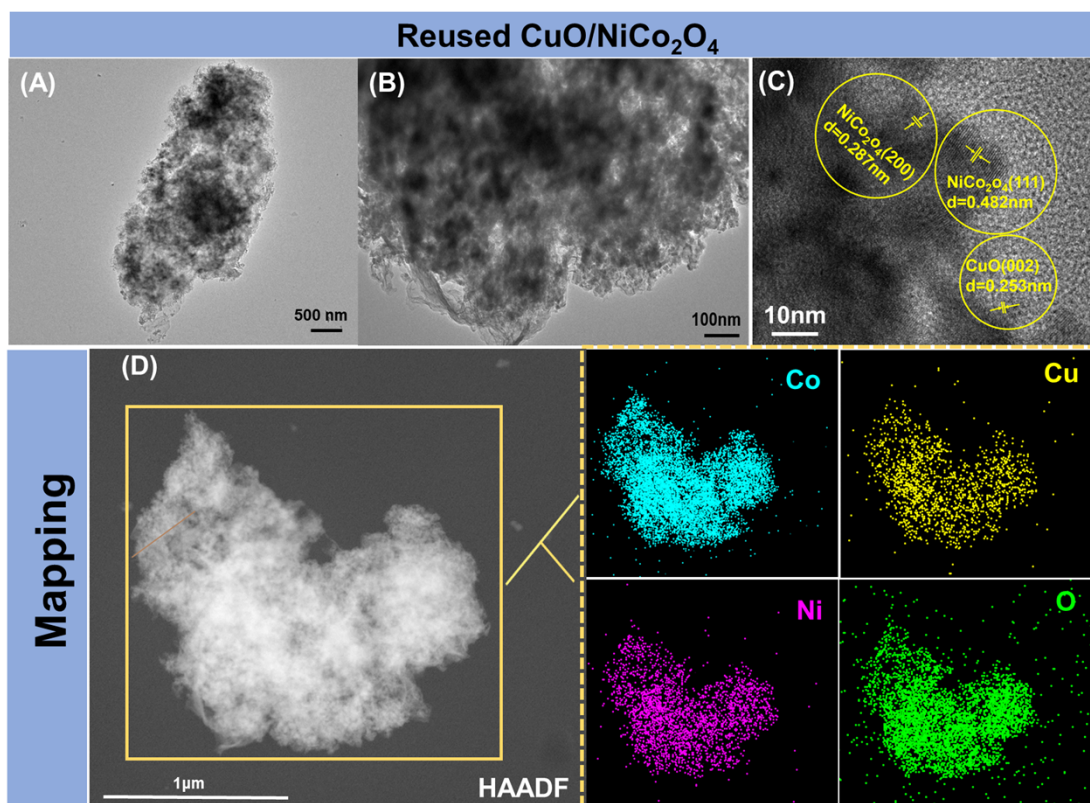


Fig. S1 TEM images (A-B), HR-TEM image (C), the element mapping (D) of reused CuO/NiCo₂O₄.

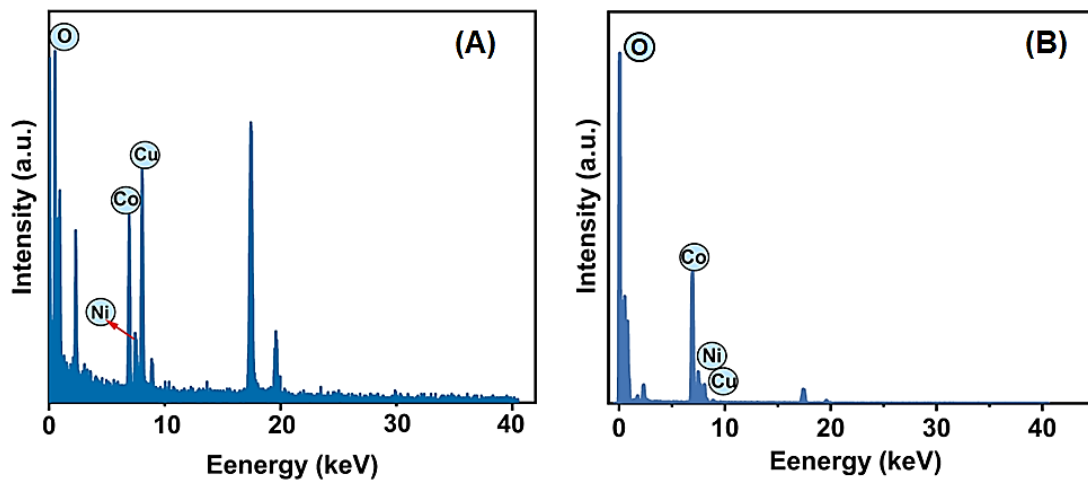


Fig. S2 EDS energy spectra of the fresh CuO/NiCo₂O₄ (A) and the reused one (B).

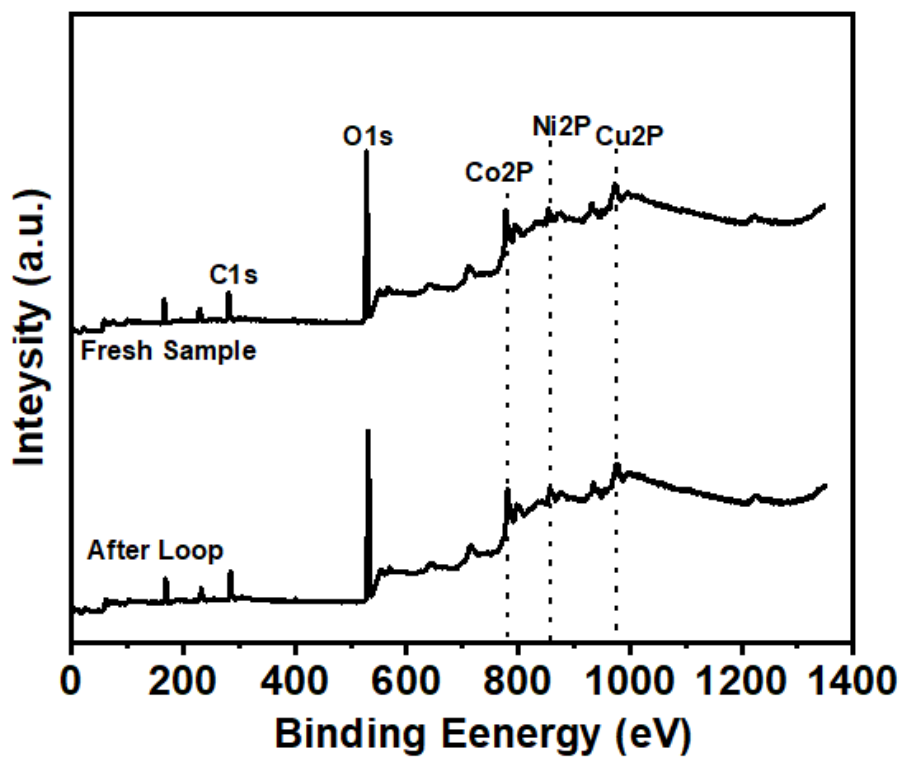


Fig. S3 XPS full spectrum of CuO/NiCo₂O₄.

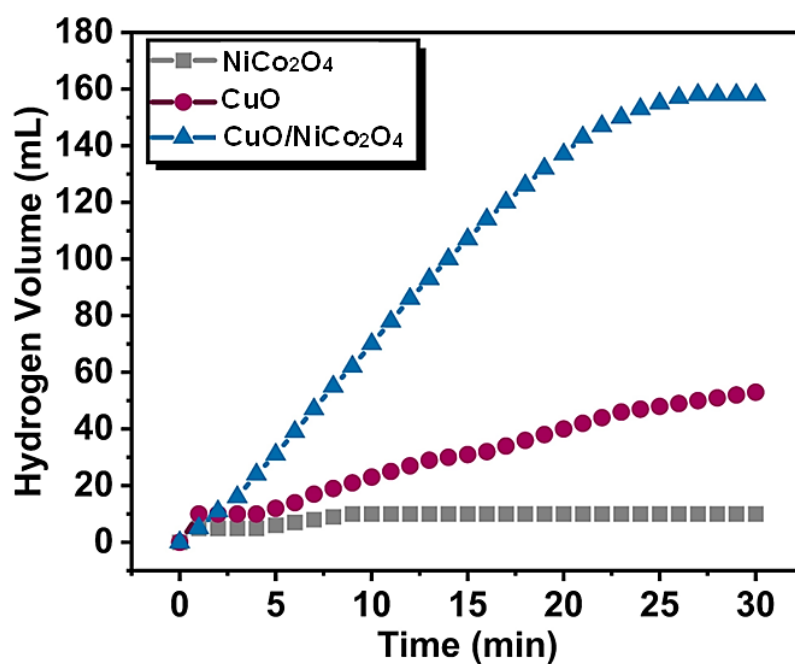


Fig. S4 Hydrogen production behaviors from AB dehydrogenation catalyzed by CuO/NiCo₂O₄, NiCo₂O₄ and CuO, respectively. Conditions: 25 °C, 30 min, 20 mg Catalyst, 2 mmol AB, 5 mL solvent (CH₃OH:H₂O = 3: 2).

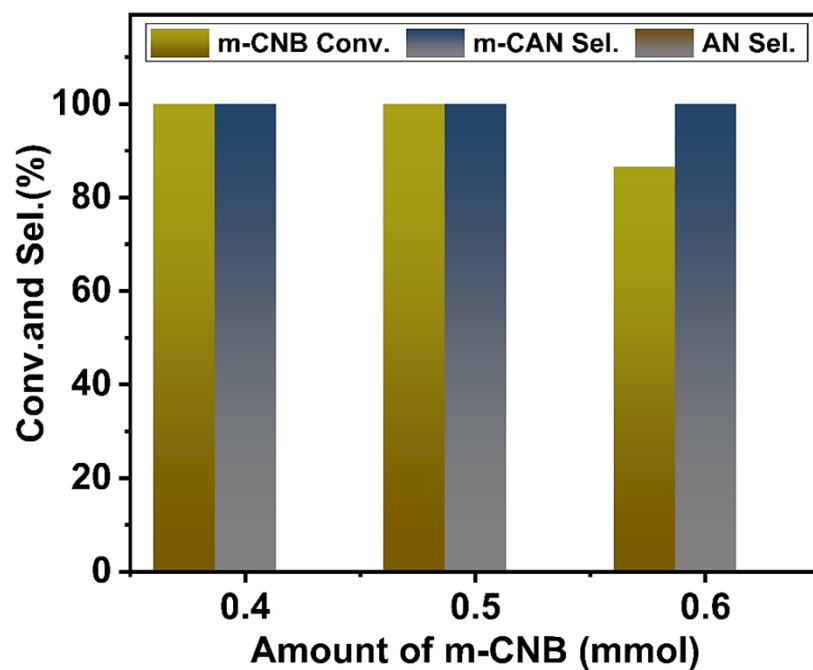


Fig. S5 Effect of the amount of m-CNB on the in situ m-CNB hydrogenation over CuO/NiCo₂O₄ in the presence of AB. Conditions: 25°C, 30 min, 20 mg CuO/NiCo₂O₄, 2 mmol AB, 5 mL solvent (CH₃OH:H₂O = 3: 2).

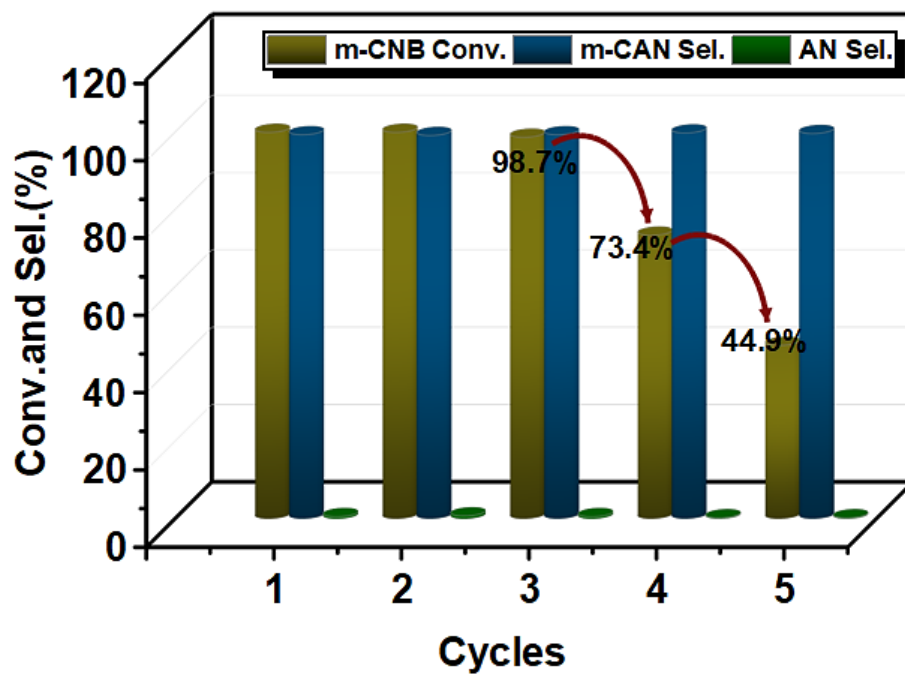


Fig. S6 Cyclic experiment of sole CuO. Conditions: 25°C, n_{AB} = 2 mmol, n_{m-CNB} = 0.5 mmol, $m_{cat.}$ = 20 mg, $V_{solvent}$ = 5 mL (CH₃OH : H₂O = 3:2)

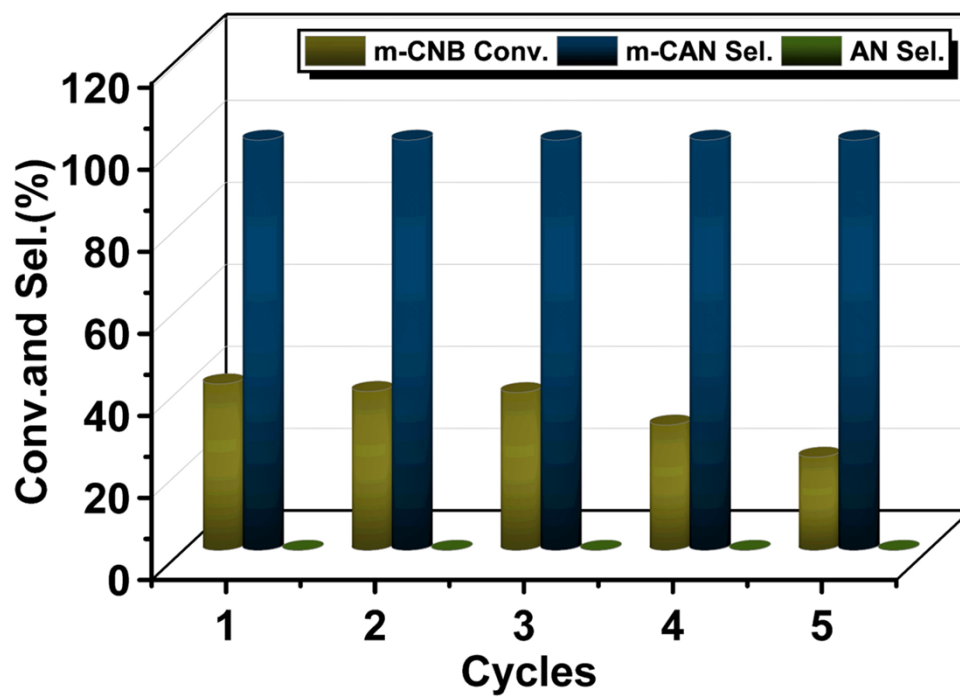


Fig. S7 Cyclic experiment of NiCo_2O_4 . Conditions: 25°C , $n_{\text{AB}} = 2 \text{ mmol}$, $n_{\text{m-CNB}} = 0.5 \text{ mmol}$, $m_{\text{cat.}} = 20 \text{ mg}$, $V_{\text{solvent}} = 5 \text{ mL}$ ($\text{CH}_3\text{OH} : \text{H}_2\text{O} = 3:2$)

Table S1. Surface compositions of the fresh and reused CuO/NiCo₂O₄ sample

Element	Fresh Sample Atomic/%	Reused Sample Atomic/%
O1s	79.98	81.49
Co2p	12.05	11.26
Ni2p	4.48	5.13
Cu2p	3.49	2.12

Note: Data listed here are estimated from XPS determination. C 1s atom % is not shown here because it does not belong to bulk catalyst sample.

Table S2. Comparison of tandem hydrogenation of m-chloronitrobenzene (m-CNB) catalyzed by different catalysts ^a

Entry	Catalyst	Conv.	Sel.	
			m-CAN	AN
1	NiCo ₂ O ₄	40.7	100	0
2	CuO	99.2	99.7	0.8
3 ^b	NiCo ₂ O ₄ + CuO	81.7	100	0
4	CuO/NiCo ₂ O ₄	100	100	0

Reaction conditions: a 25 °C, n_{m-CNB} = 0.5 mmol, n_{AB} = 2 mmol, m_{cat.} = 20 mg, 5 mL solvent (CH₃OH:H₂O = 3:2); b 25 °C, n_{m-CNB} = 0.5 mmol, n_{AB} = 2 mmol, m_{cat.} = 20 mg (NiCo₂O₄, 10 mg; CuO, 10 mg), 5 mL solvent (CH₃OH:H₂O = 3:2)

Table S3. ICP-OES data for fresh and reused CuO/NiCo₂O₄ samples.

Entry	Catalyst	Co(wt%)	Ni(wt%)	Cu(wt%)
1	Fresh CuO/NiCo ₂ O ₄	14.6	4.30	35.2
2	Reused CuO/NiCo ₂ O ₄	34.0	18.1	23.7