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Supporting Information

Experimental and Computational Studies on Copper-Cerium Catalysts Supported on Nitrogen-Doped Porous Carbon for Preferential Oxidation of CO

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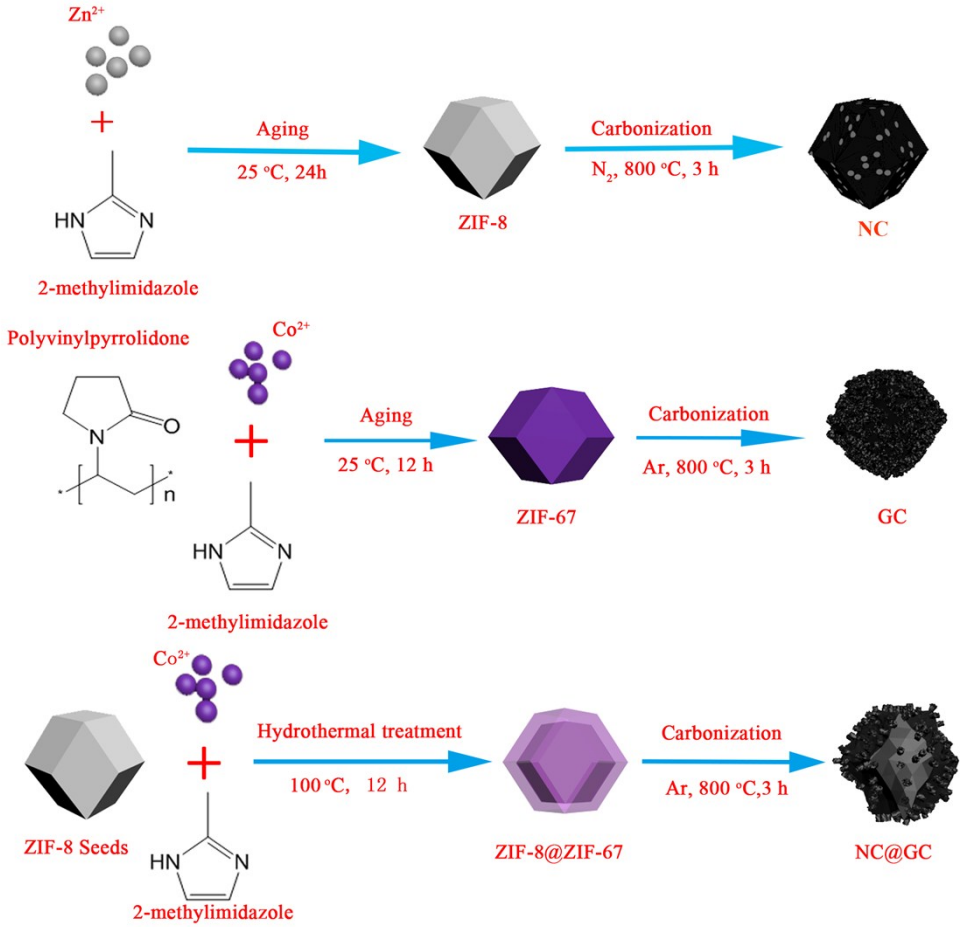

Scheme 1. Schematic synthesis processes of the NC, GC and NC@GC supports.

Table S1 Structural and textural properties of the supports.

Support	I_D/I_G	S_{BET} (m^2/g)
NC	1.11	694.57
GC	1.08	261.61
NC@GC	1.08	360.06

Table S2 Comparison of catalytic performance over the CuCe/NC, CuCe/GC, CuCe/NC@GC and reported copper-cerium oxide catalysts for CO-PROX

Catalysts	Operating conditions	Space velocity ($mL \cdot g_{cat}^{-1} \cdot h^{-1}$)	T_{50}[a] (°C)	T_{100}[b] (°C)	CO_2-selectivity at T_{100} (%)	Width[c]	Ref.
CuCe/NC	1% CO, 1% O_2, 50% H_2 in N_2	40,000	76	115	71	80	This work
CuCe/GC	1% CO, 1% O_2, 50% H_2 in N_2.	40,000	112	155	53	40	This work
CuCe/NC@GC	1% CO, 1% O_2, 50% H_2 in N_2.	40,000	105	135	83	60	This work
CuO_x/CeO_2-RGO	1% CO,1.25% O_2,50% H_2 in He.	80,000	88	135	64	60	[4]
CuCe-S	0.5% CO, 0.9% O_2, 50% H_2 in N_2 .	66,667	86	145	70	20	[9]
CuxO-CeO_2/HPC-B	1% CO, 1% O_2, 50% H_2 in N_2.	40,000	80	115	81	80	[18]
$Cu_{0.3}Ce_{0.7}O_2$-650 °C	1% CO, 1% O_2, 50% H_2 in N_2	60,000	70	115	73	55	[S1]
CuCeO-ETH	1% CO, 1% O_2, 50% H_2 in Ar .	18,000	73	100	100	95	[S2]
$Cu_{2.5}Ce_{7.5}$	1% CO, 1% O_2, 50% H_2 in N_2 .	20,000	55	95	90	120	[S3]
CuCe	1% CO, 1% O_2, 60% H_2 in He.	12,0000	98	155	55	45	[S4]
Cu(K)/CeO_2/CNT	1% CO, 1% O_2, 50% H_2 in He.	12,0000	112	175	70	25	[S5]

T_{50}[a]: Temperature at 50% CO conversion; T_{100}[b]: Temperature at 100% CO conversion; Width[c]: Width of temperature window (CO conversion > 99.0%)

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[S2] X. D. Zhang, X. L. Zhang, L. Song, F. L. Hou, Y. Q. Yang, Y. X. Wang, N. Liu, *Int. J. Hydrogen Energ.*, 2018, 43, 18279-18288.

[S3] T. Y. Kou, C. H. Si, J. Pinto, C. Y. Ma, Z. H. Zhang, *Nanoscale*, 2017, 9, 8007-2014.

[S4] J. L. Ayastuy, E. Ferna´ndez-Puertas, M. P. Gonza´lez-Marcos and M. A. Gutie´rrez-Ortiz, *Int. J. Hydrog. Energy*, 2012, **37**, 73-85.

[S5] A. B. Dongil, B. Bachiller-Baeza, E. Castillejos, N. Escalona, A. Guerrero-Ruiz, I. Rodríguez-Ramos, *Catal. Today*, 2018, 301, 141-146.

Table S3 N content for the fresh and used CuCe/NC-400 catalysts

Catalysts	Pyridine-N (%)	N content
fresh-CuCe/NC	74.00	5.56
used-CuCe/NC	62.04	1.72

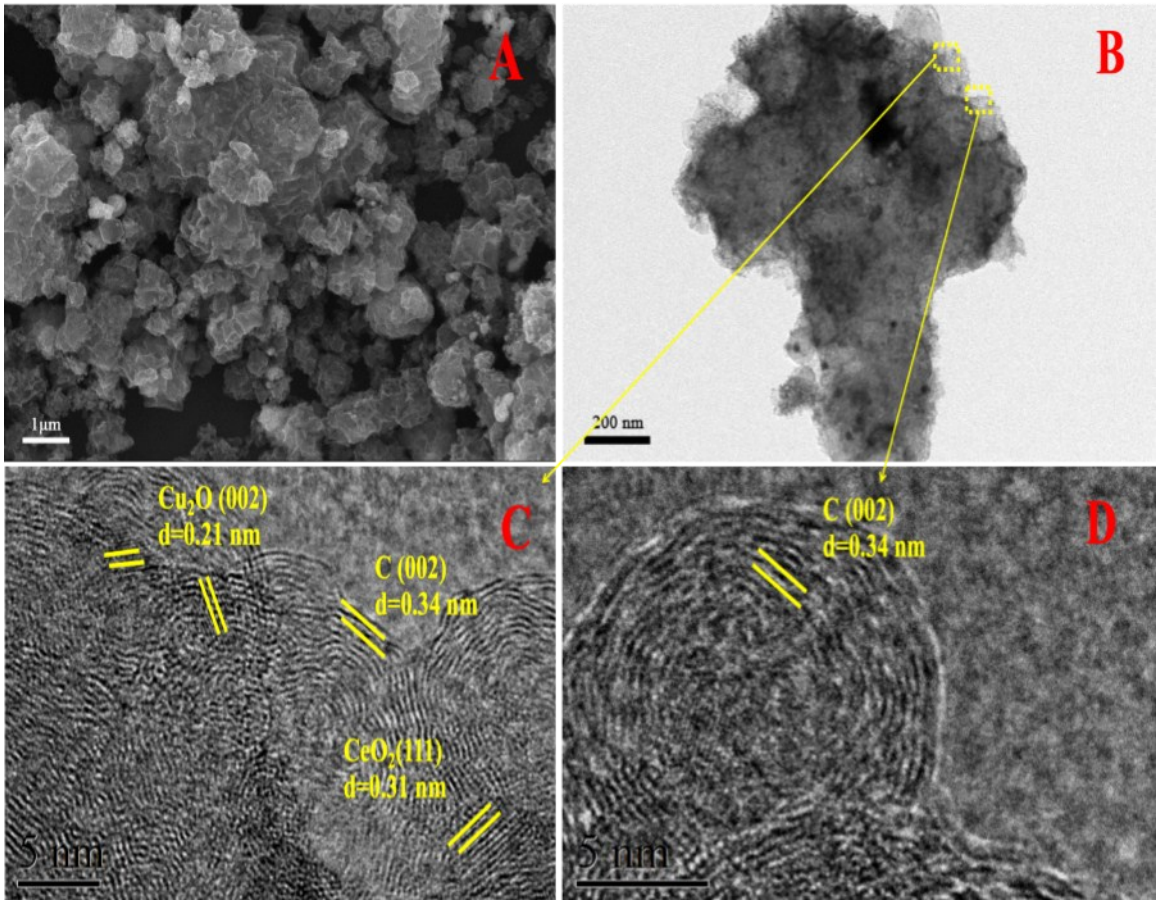

Fig. S1 SEM and TEM images of the CuCe/NC@GC catalyst.

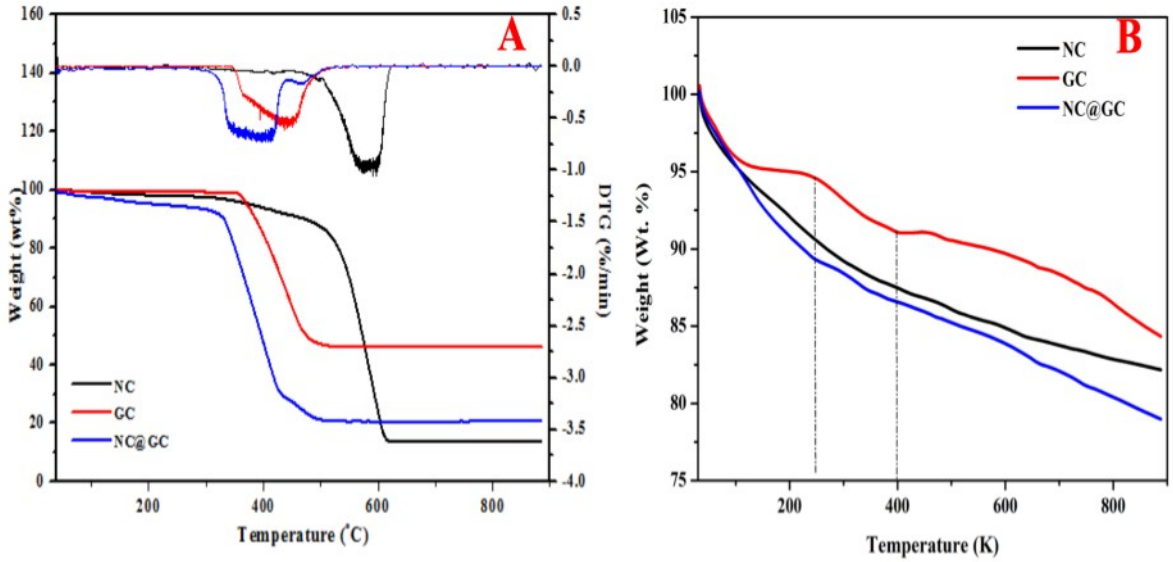

Fig. S2 TG curves of the carbon supports in (A) air and (B) N_2 atmosphere.

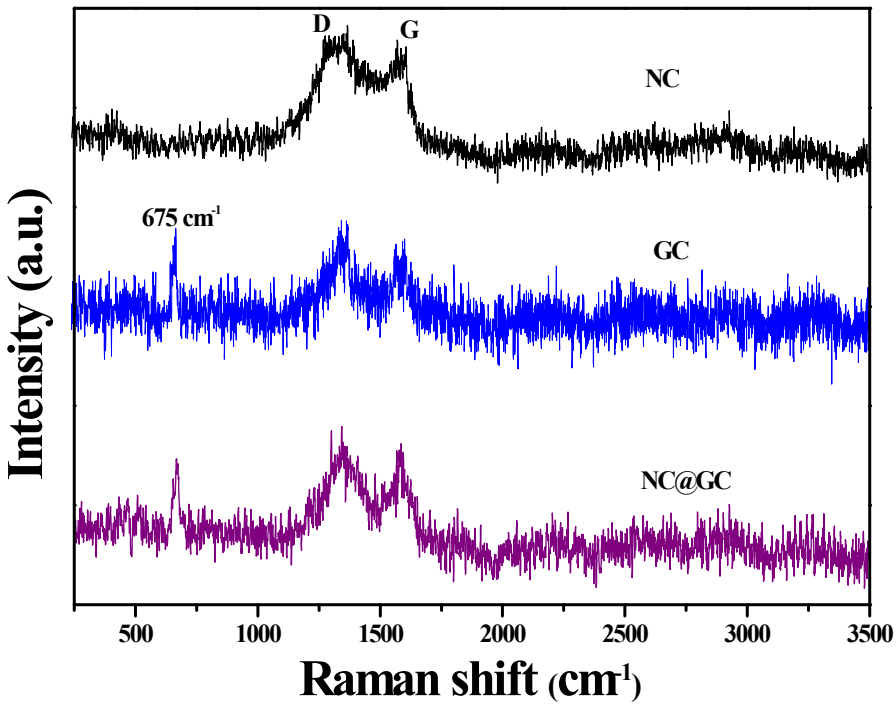

Fig. S3 Raman spectra of the supports.

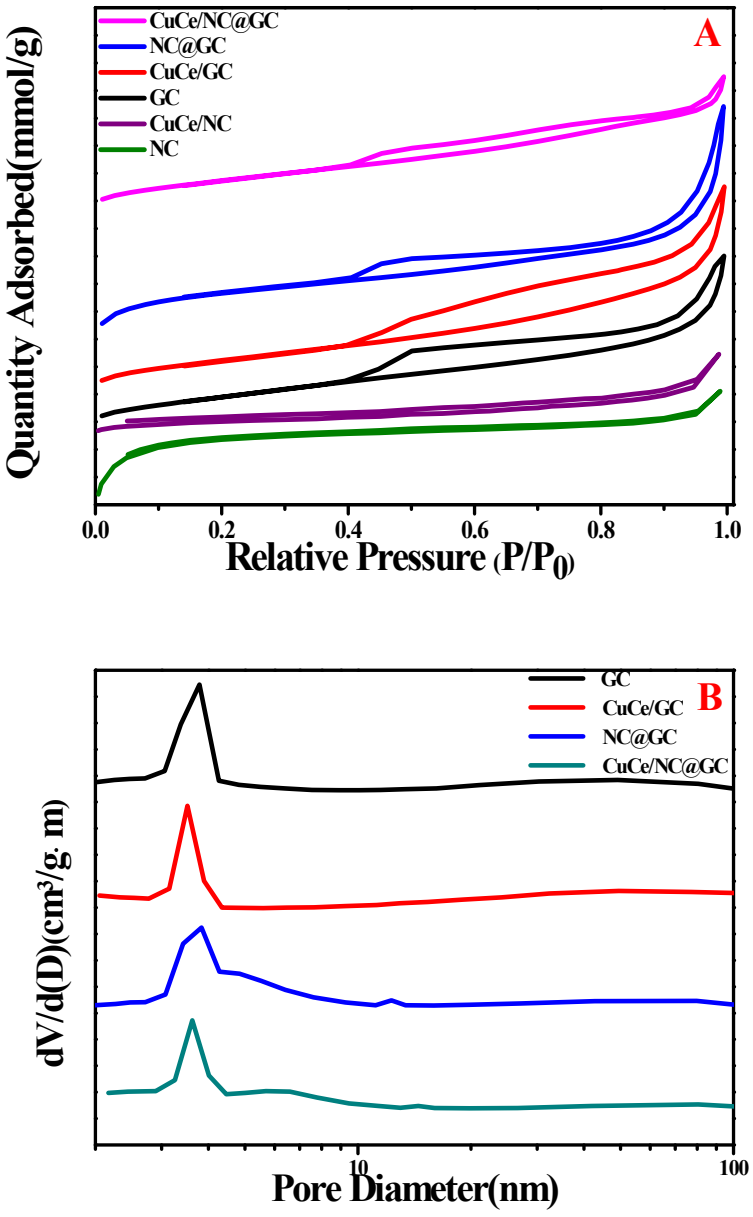

Fig. S4 (A) N_2 adsorption-desorption isotherms and (B) BJH pore size distribution curves of the supports and catalysts.

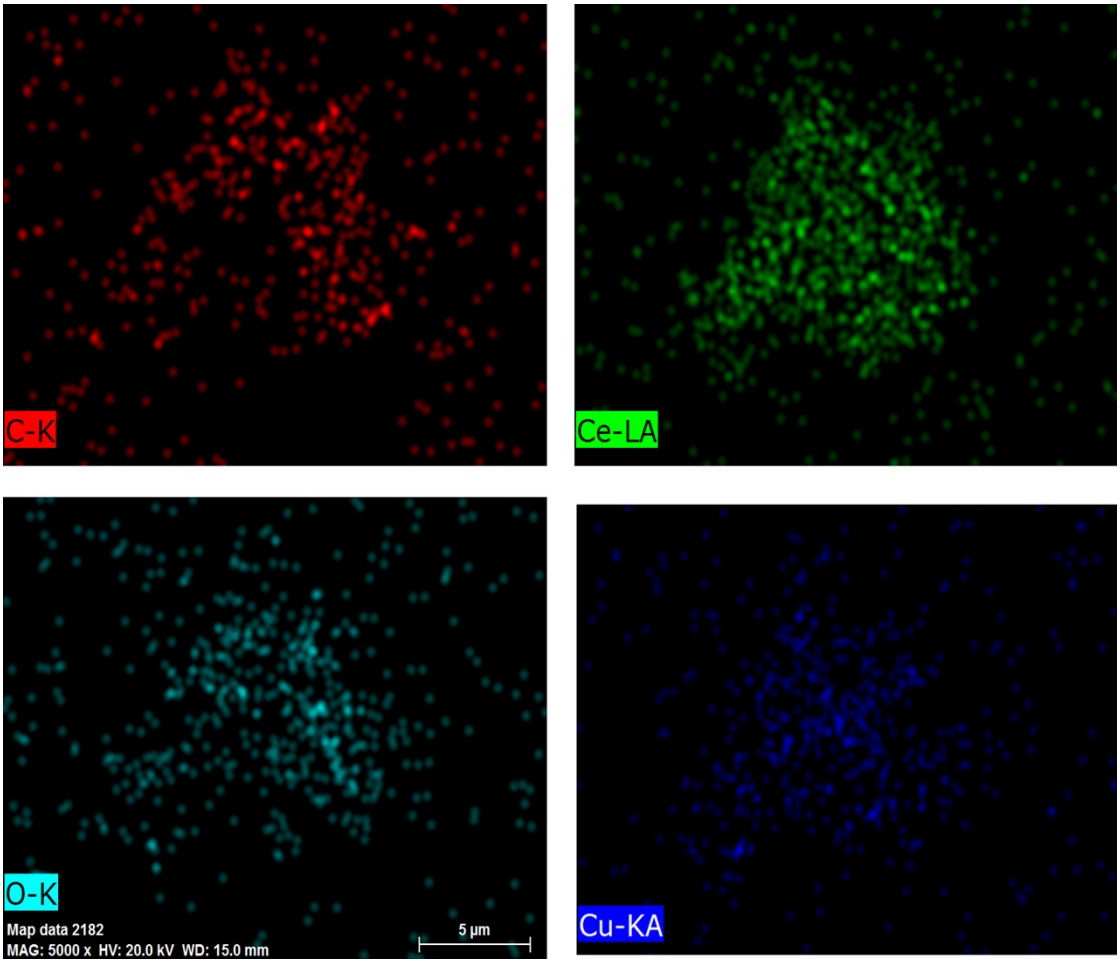

Fig. S5 EDS mapping images of the CuCe/NC-400 catalyst.

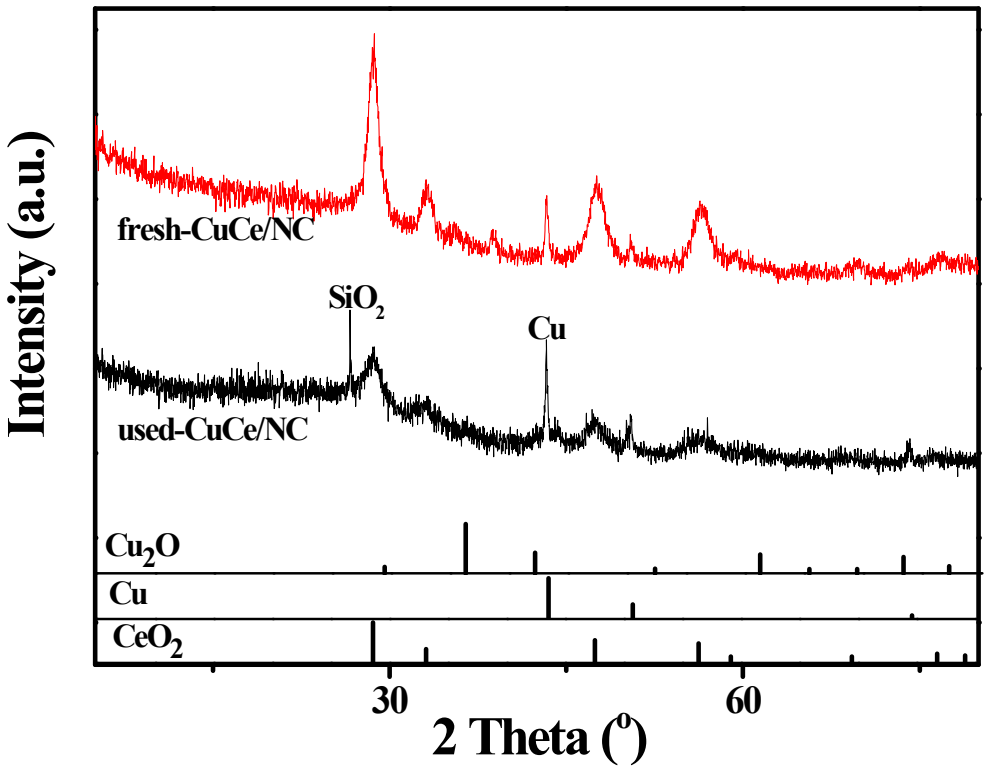

Fig. S6 XRD patterns of the fresh and used CuCe/NC-400 catalysts

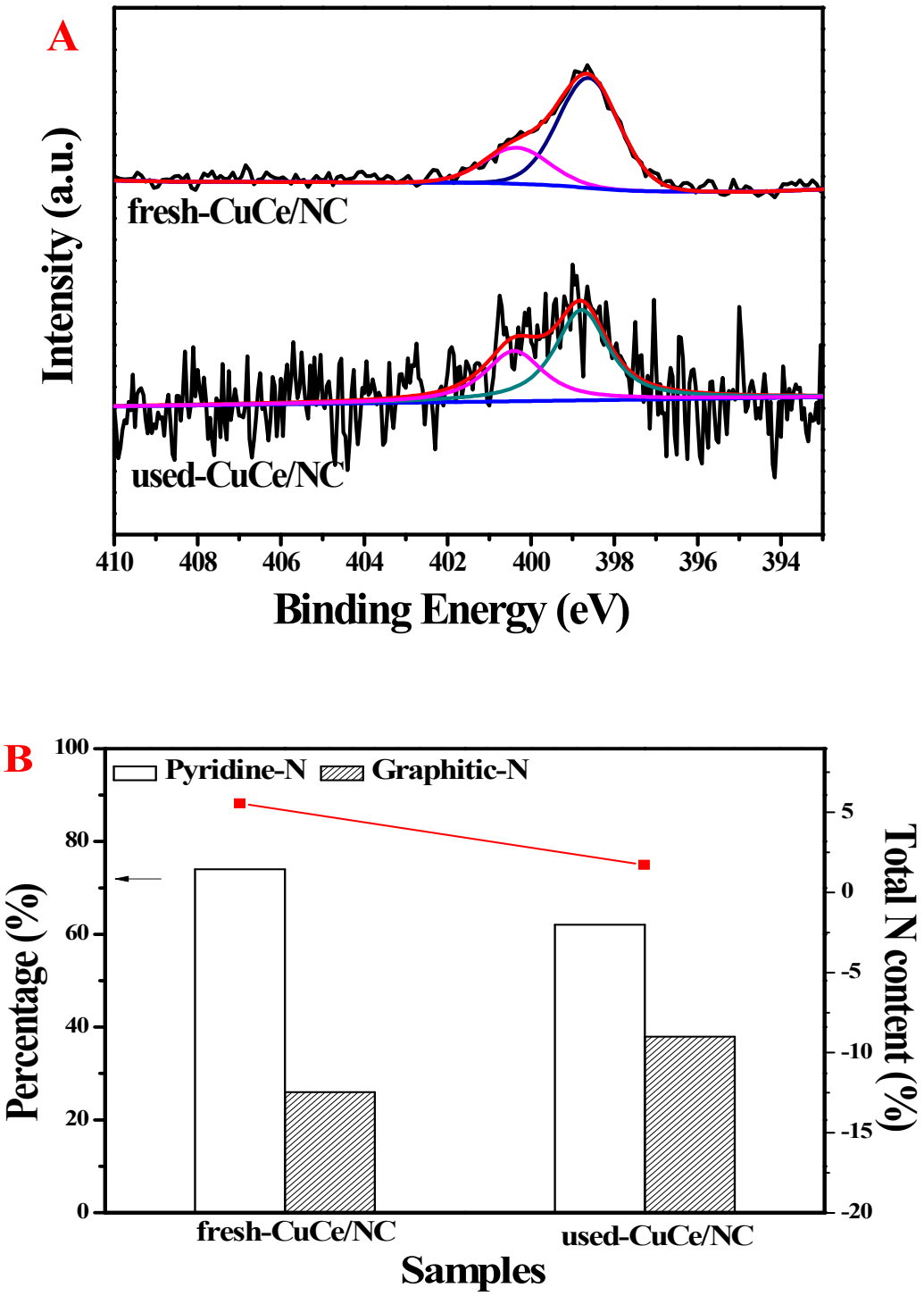

Fig. S7 XPS spectra and analyses of N content for the fresh and used CuCe/NC-400 catalysts