

Supporting Information

Selective oxidation of cyclohexane to KA oil over Co and Fe nanoparticles immobilized on layered double hydroxide nanocatalytic system

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Table S1. Influence of TBHP on cyclohexane oxidation over CoNPs@LDH nanocatalyst

Cyclohexane:TBHP (molar ratio)	Conversion (%)	Product selectivity (%)				K/A (molar ratio)	TON
		K	A	others	KA oil		
1:1	16.8	48.5	43.4	8.1	91.9	1.12	210
1:2	30.4	56.7	36.7	6.6	93.4	1.55	380
1:3	45.7	64.3	31.5	4.2	95.8	2.04	571
1:4	46.2	64.7	30.5	4.8	95.2	2.12	577

Reaction conditions: Cyclohexane (10 mmol), Catalyst (100 mg), 353 K, 6 h.

Table S2. Influence of catalyst amount on oxidation of cyclohexane over CoNPs@LDH nanocatalyst

Catalyst amount (mg)	Conversion (%)	Product selectivity (%)				K/A (molar ratio)	TON
		K	A	others	KA oil		
25	14.9	51.7	34.8	13.5	86.5	1.49	744
50	31.5	57.3	35.7	7.0	93.0	1.61	788
75	37.5	60.8	34.5	4.7	95.3	1.76	625
100	45.7	64.3	31.5	4.2	95.8	2.04	571

Reaction conditions: Cyclohexane (10 mmol), TBHP (30 mmol), 353 K, 6 h.

Table S3. Influence of temperature on oxidation of cyclohexane over CoNPs@LDH nanocatalyst

Temperature (K)	Conversion (%)	Product selectivity (%)				K/A (molar ratio)	TON
		K	A	others	KA oil		
333	26.5	46.2	41.2	12.6	87.4	1.12	331
343	36.4	51.1	40.7	8.2	91.8	1.26	455
353	45.7	64.3	31.5	4.2	95.8	2.04	571
363	45.5	64.7	30.5	4.8	95.2	2.12	569

Reaction conditions: Cyclohexane (10 mmol), TBHP (30 mmol), Catalyst (100 mg), 6 h.

Table S4. Comparison of reference catalysts with our catalyst system for cyclohexane oxidation with TBHP under solvent-free condition

Catalyst	Oxidant	Temperature (K)	Time (h)	Conversion (%)	Selectivity of KA oil (%)	[Ref.]
Cu-MgAlO	O ₂	423	2	8.3	82.9	[10]
CoO/G	O ₂	393	6	32.4	75.4	[15]
MCoS(20)	TBHP	373	14	28.8	95.7	[50]
Co-g-C ₃ N ₄ (15)	TBHP	413	4	10.60	84.6	[51]
AgPd/MgO	O ₂	413	17	9.5	78.0	[52]
α -ZrP.Co(Salicylaldimine)TBHP		353	6	14.2	92.3	[53]
FeNPs@LDH	TBHP	353	6	27.3	92.8	This work
CuNPs@LDH	TBHP	353	6	45.7	95.8	This work

Table S5. Influence of time on oxidation of cyclohexane over CoNPs@LDH nanocatalyst

Time (h)	Conversion (%)	Product selectivity (%)				K/A (molar ratio)	TON
		K	A	others	KA oil		
0	-	-	-	-	-	-	-
1	6.4	45.6	41.8	12.6	87.4	1.09	80
2	12.7	52.4	43.3	4.3	95.7	1.21	159
4	34.8	58.1	37.6	4.3	95.7	1.55	435
6	45.7	64.3	31.5	4.2	95.8	2.04	571

Reaction conditions: Cyclohexane (10 mmol), TBHP (30 mmol), Catalyst (100 mg), Temperature 353 K

Table S6. Recyclability of CoNPs@LDH nanocatalyst for the oxidation of cyclohexane

Entry	Number of Runs	Conversion (%)	Selectivity of KA oil (%)
1	Fresh catalyst	45.78	95.8
2	1	45.7	95.8
3	2	45.7	95.8
4	3	45.3	95.7
5	4	44.9	95.7

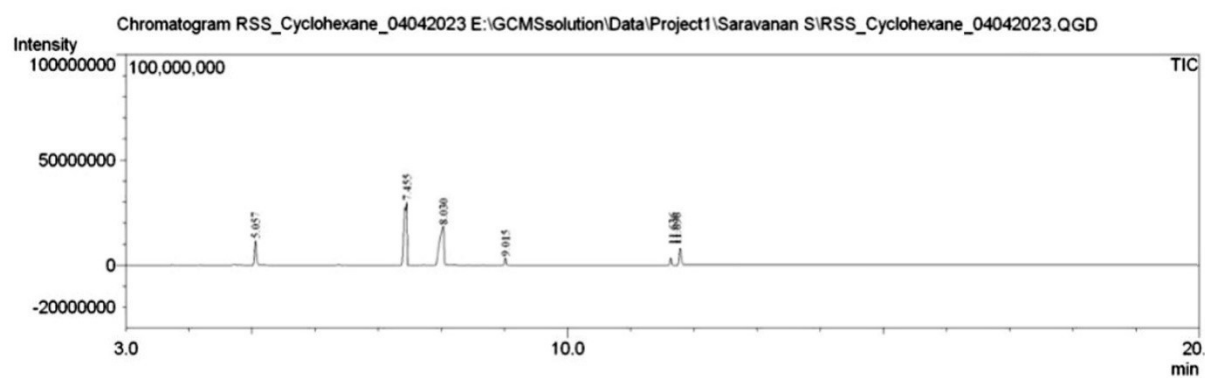
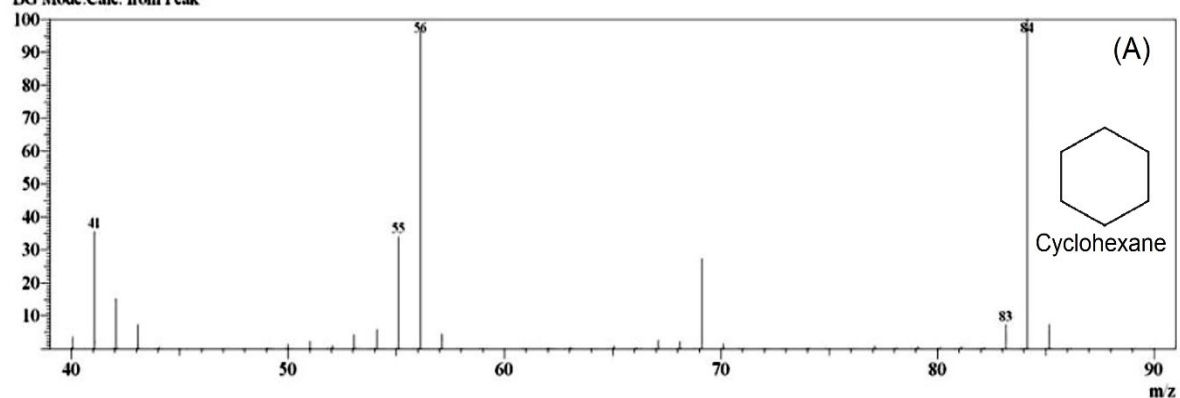
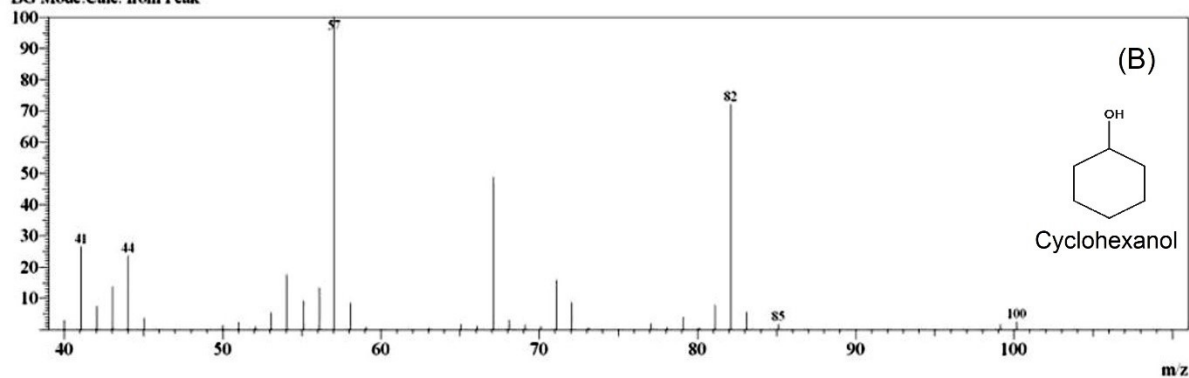


Figure S1. GC-MS chromatogram of reaction mixture of cyclohexane oxidation

Line#:2 R.Time:7.5(Scan#:896)
MassPeaks:41
RawMode:Averaged 7.5-7.5(895-897) BasePeak:84(5333022)
BG Mode:Calc. from Peak



Line#:5 R.Time:11.6(Scan#:1397)
MassPeaks:36
RawMode:Averaged 11.6-11.6(1396-1398) BasePeak:57(283168)
BG Mode:Calc. from Peak



Line#:6 R.Time:11.7(Scan#:1405)
MassPeaks:26
RawMode:Averaged 11.7-11.7(1404-1406) BasePeak:55(316617)
BG Mode:Calc. from Peak

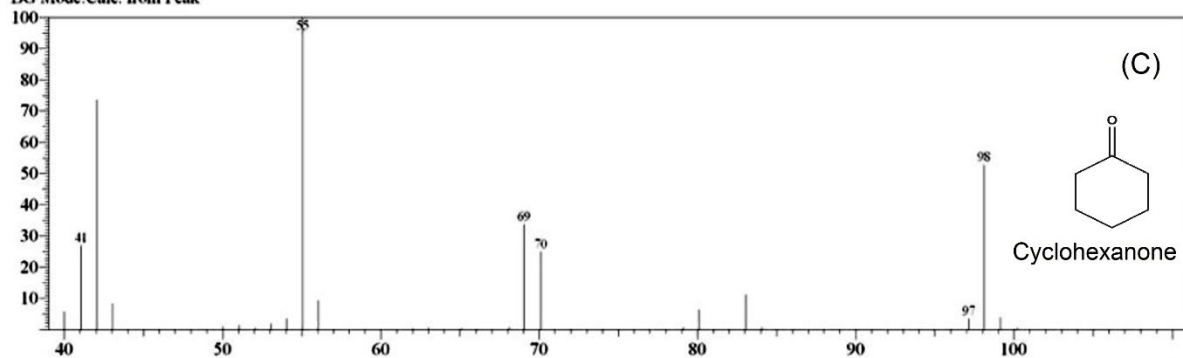


Figure S2. Mass spectra of (A) cyclohexane, (B) cyclohexanol and (C) cyclohexanone

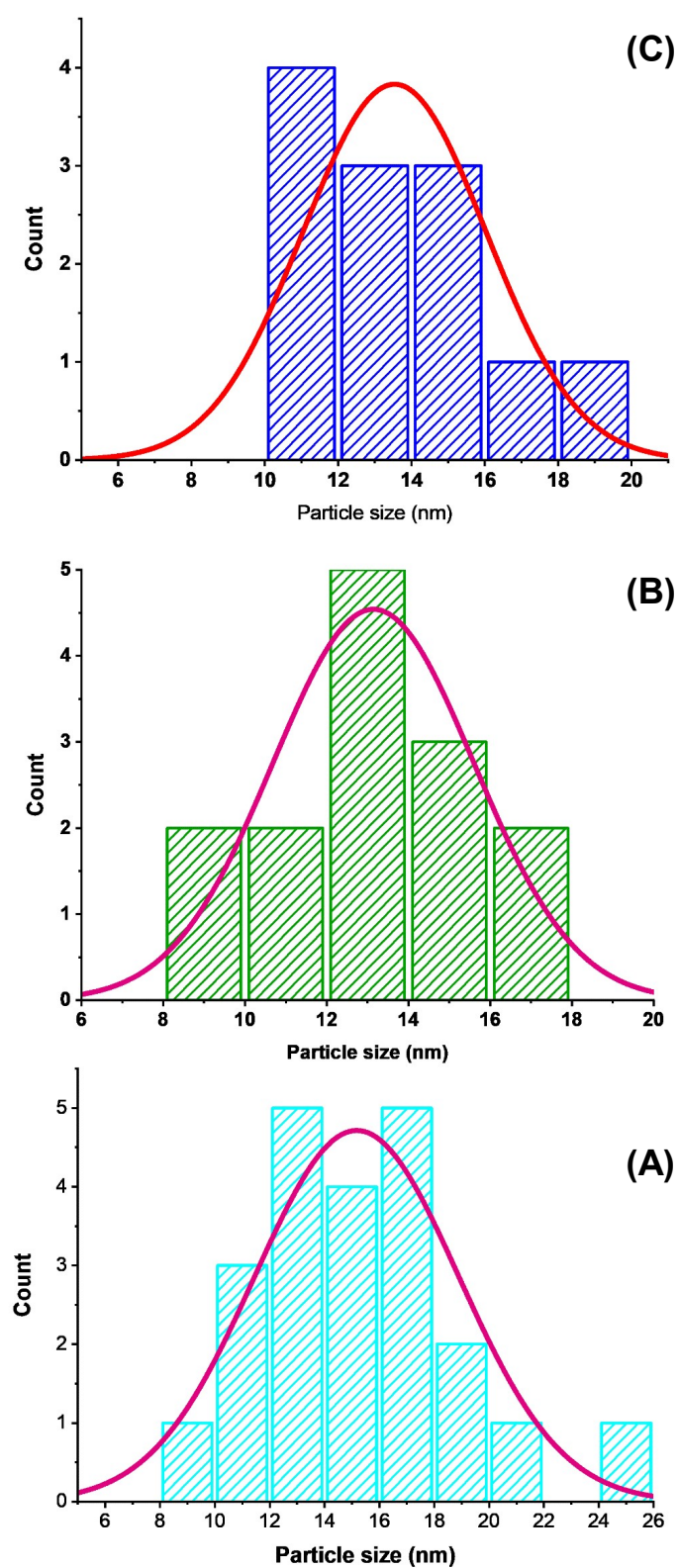


Figure S3. Average particle size histogram of (a) LDH-[OH-C₆H₄COO], (b) FeNPs@LDH, and (c) CoNPs@LDH

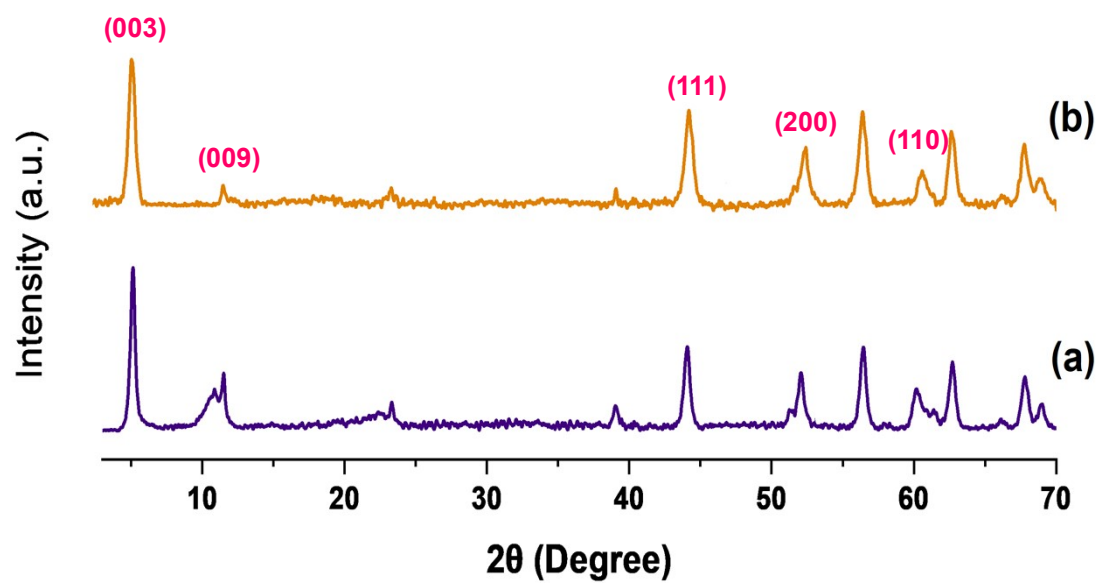


Figure S4. XRD pattern of (a) fresh CoNPs@LDH (b) reused CoNPs@LDH

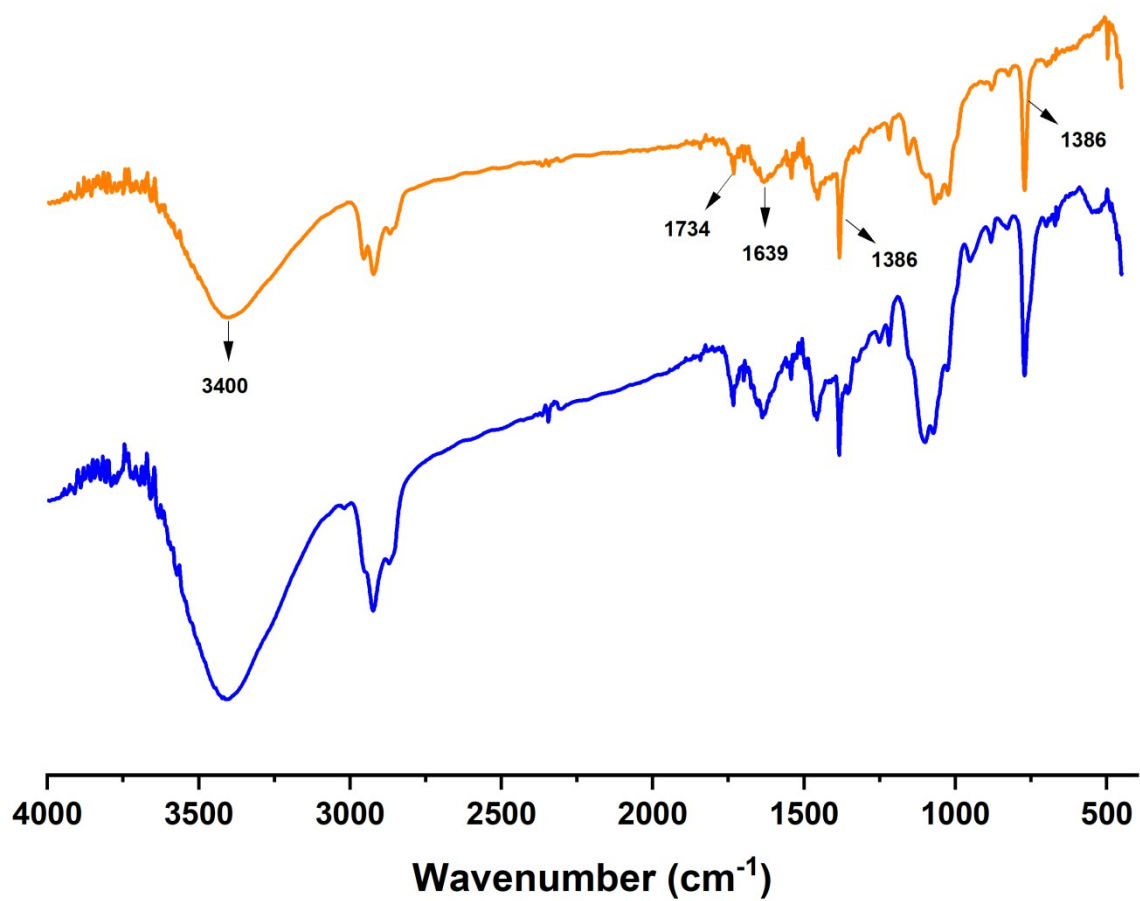


Figure S5. FTIR spectra of (a) fresh CoNPs@LDH (b) reused CoNPs@LDH