Electronic Supplementary Material (ESI) for Green Chemistry.

Nitrogen-doped carbon modified nickel catalyst for the hydrogenation of levulinic acid under mild conditions

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Table S1. Comparison of reaction conditions of hydrogenation of levulinic acid over different nickel-based catalysts.

Entry	Catalyst	Ni content (wt. %)	Reaction conditions	Selectivity (%)	Ref.
1	Ni/MgO	44	150 ℃, 1 MPa H_2	93.3	1
2	$Ni/Mg_2Al_2O_5$	40	160 ℃, 3 MPa H_2	99.7	2
3	$Ni/\gamma\text{-}Al_2O_3$	40	180 ℃, 3 MPa H_2	98.2	3
4	Ni/NCMs	6.3	200 ℃, 3 MPa H_2	99	4
5	Ni/Al_2O_3	15	200 ℃, 5 MPa H_2	100	5
6	Ni/C-500	58.4	200 ℃, 1 MPa H_2	98.2	6
7	NiAl-LDH	7	200 ℃, 3 MPa H_2	100	7
8	Ni–MoOx/C	10	140 ℃, 8 bar H_2	97	8
9	Ni/Al_2O_3-CN-600	7.9	130 ℃, 1 bar H_2	> 99	This work

Table S2. Metal content of Ni/Al_2O_3-CN-T measured by ICP-OES.

Entry	Catalyst	Ni Content (wt %)
1	Ni/Al_2O_3-CN-500	7.1
2	Ni/Al_2O_3-CN-600	7.9
3	Ni/Al_2O_3-CN-700	8.3

Table S3. Surface atomic composition of Ni/Al_2O_3-CN-T measured by XPS.

Entry	Catalyst	Surface atomic composition (%)			
		Ni	Al	C	N
1	Ni/Al_2O_3-CN-500	1.29	25.0	26.1	0.7
2	Ni/Al_2O_3-CN-600	1.23	25.9	25.3	0.6
3	Ni/Al_2O_3-CN-700	0.93	27.3	23.9	0.4

Table S4. Textural and structural properties of NiO/Al_2O_3-CN-air and Ni/Al_2O_3-CN-T catalysts.

catalyst	Surface area (m^2/g)	Pore volume (cm^3/g)	Pore diameter (nm)
NiO/Al_2O_3-CN-air	67.70	0.10	5.91
Ni/Al_2O_3-CN-500	240.29	0.18	4.54
Ni/Al_2O_3-CN-600	162.79	0.20	4.78
Ni/Al_2O_3-CN-700	145.12	0.20	5.49

Table S5. The effect of the reaction solvents on the hydrogenation of levulinic acid over different solvents.

Entry	Catalyst	Solvent	Conv.	Sele.	Ref.
1	Ru_3TPA	Methanol	92%	75%	9
		Ethanol	91%	68%	
		Isopropanol	65%	61%	
		Butanol	52%	50%	
		Dioxane	95%	100%	
		H_2O	80%	90%	
2	CuPS-R_{350}-C_8-R_{350}	THF	95.7%	89.0%	10
		Ethanol	81.6%	90.0%	
		Water	45.5%	89.0%	
3	Ru-TS	THF	61%	0%	11
		Methanol	95%	62%	
		Ethanol	98%	86%	
		Butanol	80%	76%	
		Dioxane	21%	5%	
4	Ru/TiO_2-n	H_2O	>99%	>99%	12

		Methanol	63%	32.8%	
		Ethanol	28%	>99%	
		Dioxane	0%	0%	
5	$CuNi@SiO_2$	THF	≈82%	-	13
		H_2O	≈58%	-	
		Isopropanol	99%	96.8%	
		Dioxane	≈38%		
6	Ni–MoO_x/C	Toluene	24%	87.5%	8
		Dioxane	13%	30.8%	
		H_2O	2%	100%	
		No solvent	100%	97%	
7	$Ni_{4.59}Cu_1Mg_{1.58}Al_{1.96}Fe_{0.70}$	Water	67.5%	67.5%	14
		Methanol	98.1%	98.1%	
8	Ni/MgO	H_2O	≈2%	≈99%	1
		Methanol	≈ 80%	≈3%	
		Ethanol	≈52%	≈30%	
		isopropanol	100%	93.3%	
		Dioxane	≈89%	≈96%	
9	Ni-Sn(1.4)/AlOH	THF	21%	95%	15
		H_2O	>99%	>99%	
		Methanol	14%	0%	
		Ethanol	20%	0%	
		Isopropanol	10%	0%	
		Dioxane	35%	97.1%	

10	Ru/N@CNTs	THF	14.7%	0%	16
		H_2O	69.2%	99%	
		Methanol	40.4%	22%	
		Ethanol	20%	35.5%	
		Isopropanol	12.1%	90%	
		Dioxane	21.9%	84.9%	
11	Ni/Al_2O_3-CN-600	THF	>99%	>99%	This work
		H_2O	96.2%	98.2%	
		Toluene	93.7%	97.3%	
		Methanol	>99%	86.6%	
		Ethanol	>99%	96.1%	
		Isopropanol	93.6%	98.2%	
		Dioxane	82.1%	96.6%	

Table S6. Ni contents of Ni/Al_2O_3 before and after recycle measured by ICP-OES.

Entry	Sample	Ni contents (wt %)
1	Fresh Ni/Al_2O_3-CN-600	7.9
2	Ni/Al_2O_3-CN-600 after 5 runs	7.7
3	Fresh Ni/Al_2O_3	9.4
4	Ni/Al_2O_3 after 5 runs	7.0

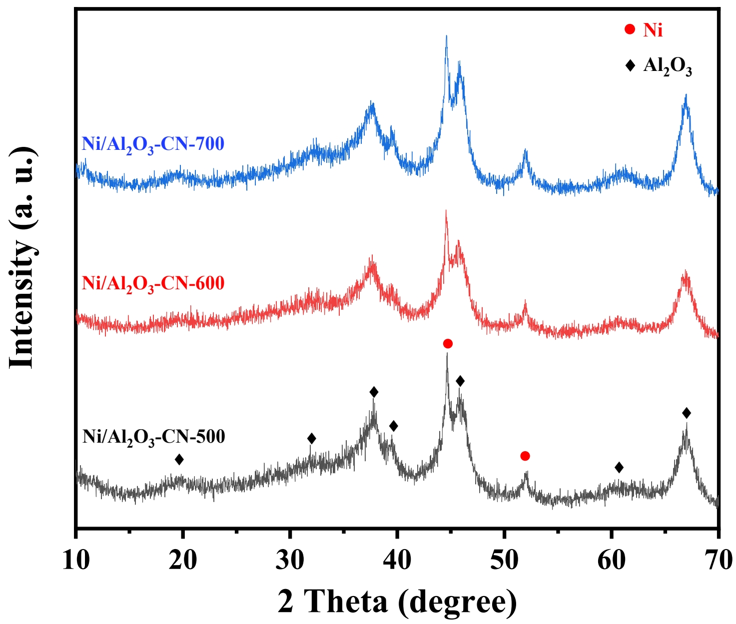

Figure S1. XRD pattern of the different Ni/Al_2O_3-CN-T catalysts.

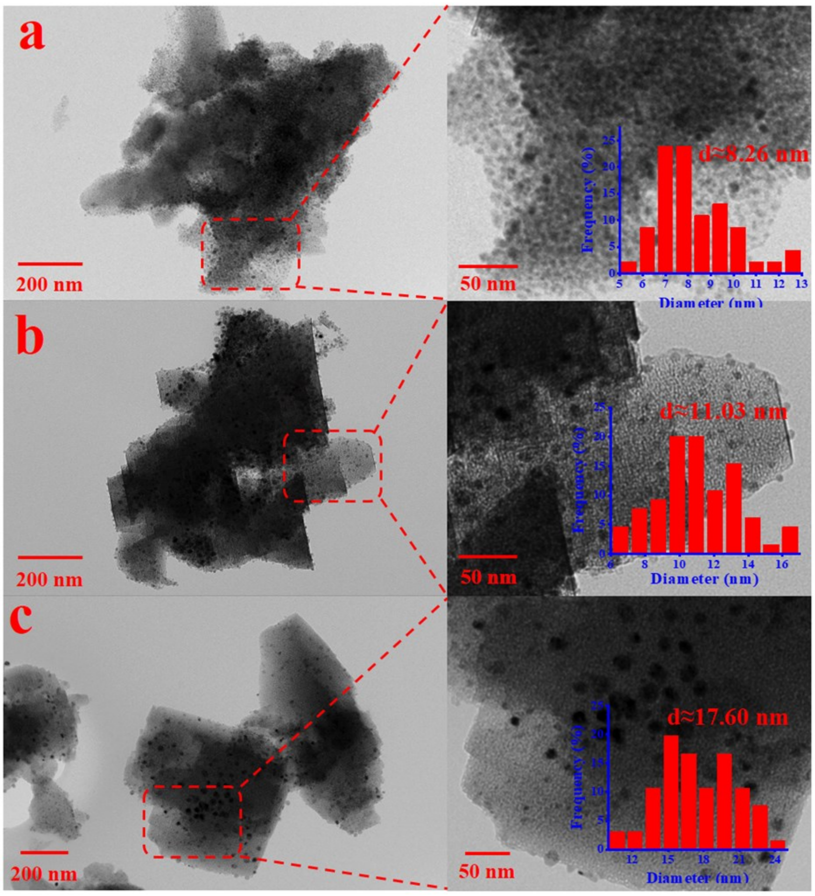

Figure S2. TEM images and average size distribution of nickel nanoparticles of the Ni/Al_2O_3-CN-500 (a), Ni/Al_2O_3-CN-500 (b) and Ni/Al_2O_3-CN-700 (c).

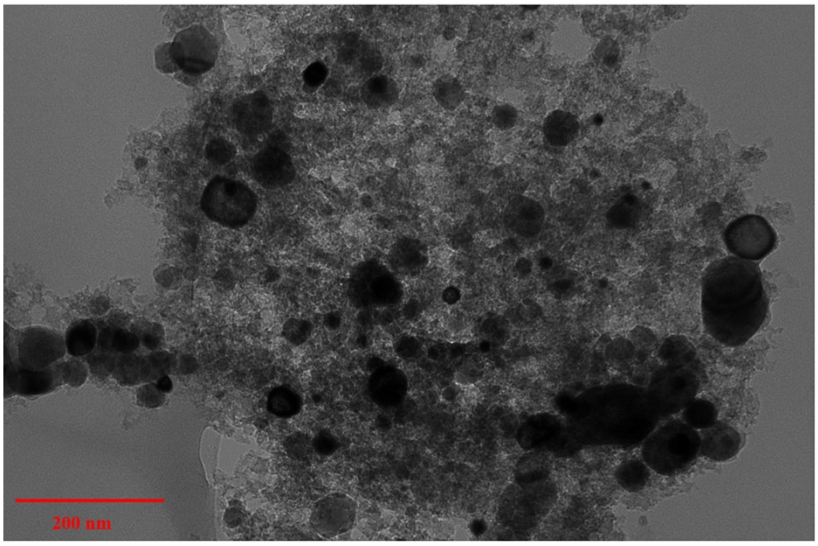

Figure S3. TEM image of Ni/CN-600.

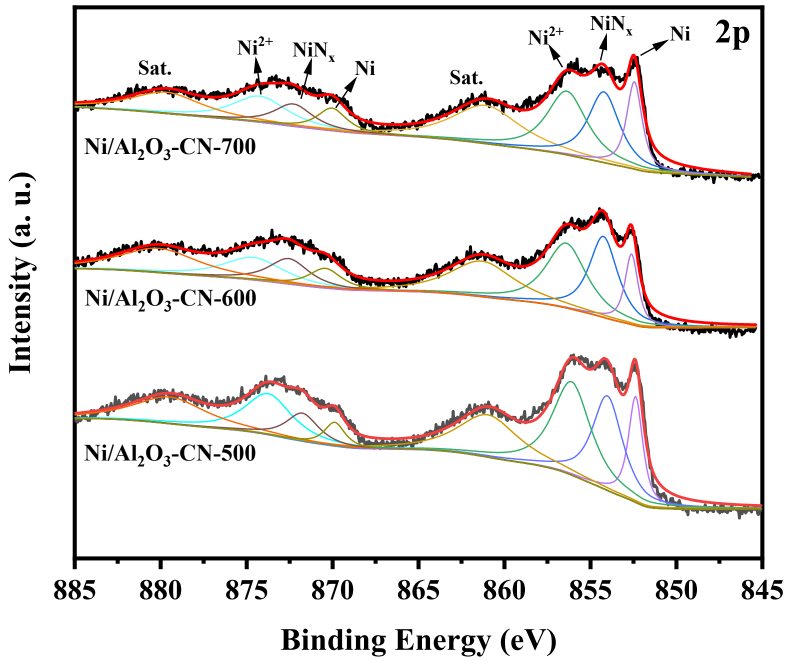

Figure S4. The Ni 2p XPS pattern of the different Ni/Al_2O_3-CN-T catalysts.

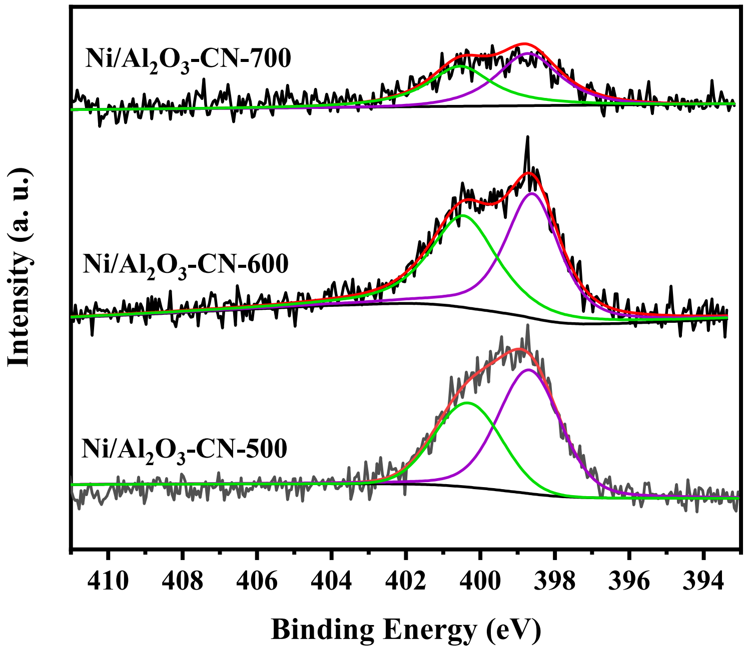

Figure S5. The N 1s XPS pattern of the different Ni/Al_2O_3-CN-T catalysts.

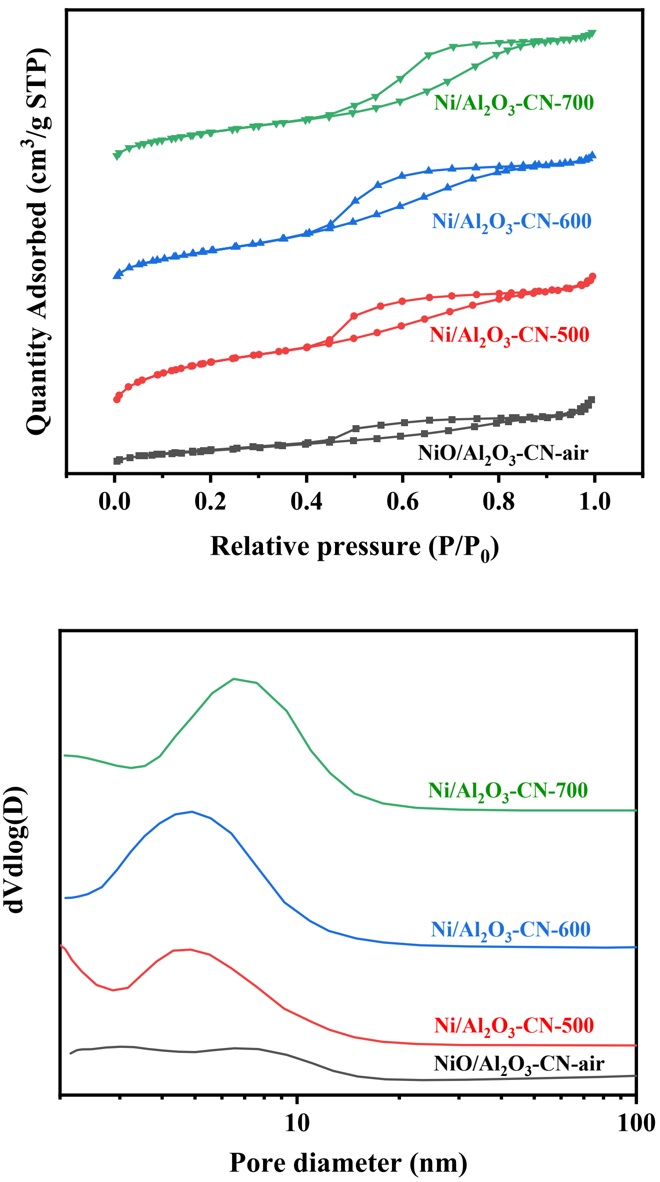

Figure S6. N_2 adsorption-desorption isotherms and pore size distributions of NiO/Al_2O_3-CN-air and the Ni/Al_2O_3-CN-T catalysts.

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