Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Supporting Information

Enhancing the anisole hydrodeoxygenation activity over Ni/Nb_2O_{5-x} by tuning the oxophilicity of the support

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Table S1. Structural properties of different Ni/Nb_2O_5-based catalysts

Catalyst	H_2 adsorption (μmol/g)[a]				H_2-consumption (μmol/g)[b]
	<200 °C	200-300 °C	>300 °C	Total	
Ni/Nb_2O_5-C	3.6 (13%)	3.4 (12%)	20.3 (75%)	27.2	423
Ni/Nb_2O_5-P	1.8 (7%)	1.0 (4%)	24.2 (89%)	27.0	390
Ni/Nb_2O_5-HT	0.8 (3%)	4.2 (14%)	25.0 (83%)	30.0	442
Ni/Nb_2O_5-H	0.7 (3%)	5.5 (24%)	16.7 (73%)	23.0	452

[a] Amount of H_2 adsorption derived from H_2-TPD, [b] H_2 consumption derived from H_2-TPR

Table S2. XPS results of the Nb 3d5/2 and O 1s of Ni/Nb_2O_5 catalysts

Catalysts[a]	Nb $3d_{5/2}$		O 1s
	Nb^{4+}/Nb^{5+}	$Nb^{4+}/Nb^{4+}+ Nb^{5+}$	O_β/ O_{total}
Ni/Nb_2O_5-C (Reduced)	0.92	0.4798	0.24
Ni/Nb_2O_5-H (Reduced)	1.01	0.504	0.35

[a] Both the catalysts were reduced ex-situ with formier gas (5% H_2 in N_2) at 400 °C for 1 h prior to the XPS analysis.

Table S3. Catalytic activity of Ni/Nb_2O_5-H and previous studies related to Ni-based catalysts for HDO of anisole

Entry	Catalysts	Reaction conditions	Conv. (%)	Selec. DeO (%)	R_{HDO} [a] (mmol. g^{-1}_{Ni}. h^{-1})*10^2	Reference
1	**3wt% Ni/Nb_2O_5**	**240 °C, 20bar H_2, 1 h**	**90**	**91.0**	**5.45**	**This work**
2	10wt% Ni/SiO_2	300 °C, 50 bar H_2, 16 h	>99	80.4	0.23	[1]
3	10wt% Ni/Al_2O_3	300 °C, 50 bar H_2, 16 h	>99	74	0.21	[1]
5	30wt% Ni/Al_2O_3-ZrO_2	230 °C, 10 bar H_2, 3 h	100	77.6	0.97	[2]
6	10wt% Ni/SiO_2	220 °C, 30 bar H_2, 4 h	>99	95	2.59	[3]
7	90wt% Ni/Nb_2O_5	240 °C, 30bar H_2, 4h	>99	100	0.38	[4]
8	60wt% Ni 5wt%Cu 30wt%Si	320 °C, 60bar H_2, 2.5h	~85	100	2.59	[5]
9	5wt% Ni/TiO_2-ZrO_2	300 °C, 40bar H_2, 4h	60	~87	5.19	[6]
10	90wt%Ni /SiO2	280 °C, 60bar H_2, 0.75h	100	40	0.12	[7]
11	16wt%Ni-2wt% Cu/Al_2O_3	300°C, 10bar H_2, continuous-flow study	78.6	95.9	-	[8]
12	20wt%Ni/TiO_2 20wt%Ni/SBA-15	310°C, 15bar H_2, WHSV=20.4^{-h}	100	~90%	-	[9]
13	10wt%Ni/SBA-15	280°C, 35bar H_2, 6h	100	100	2.98	[10]
14	5wt%Ni/HSZ	200°C, 68bar H_2, 2.3 h	98	84	3.68	[11]

[a] R_{HDO} = mol of the deoxygenated product (cyclohexane)/mass of Ni present in the catalyst * time(h)

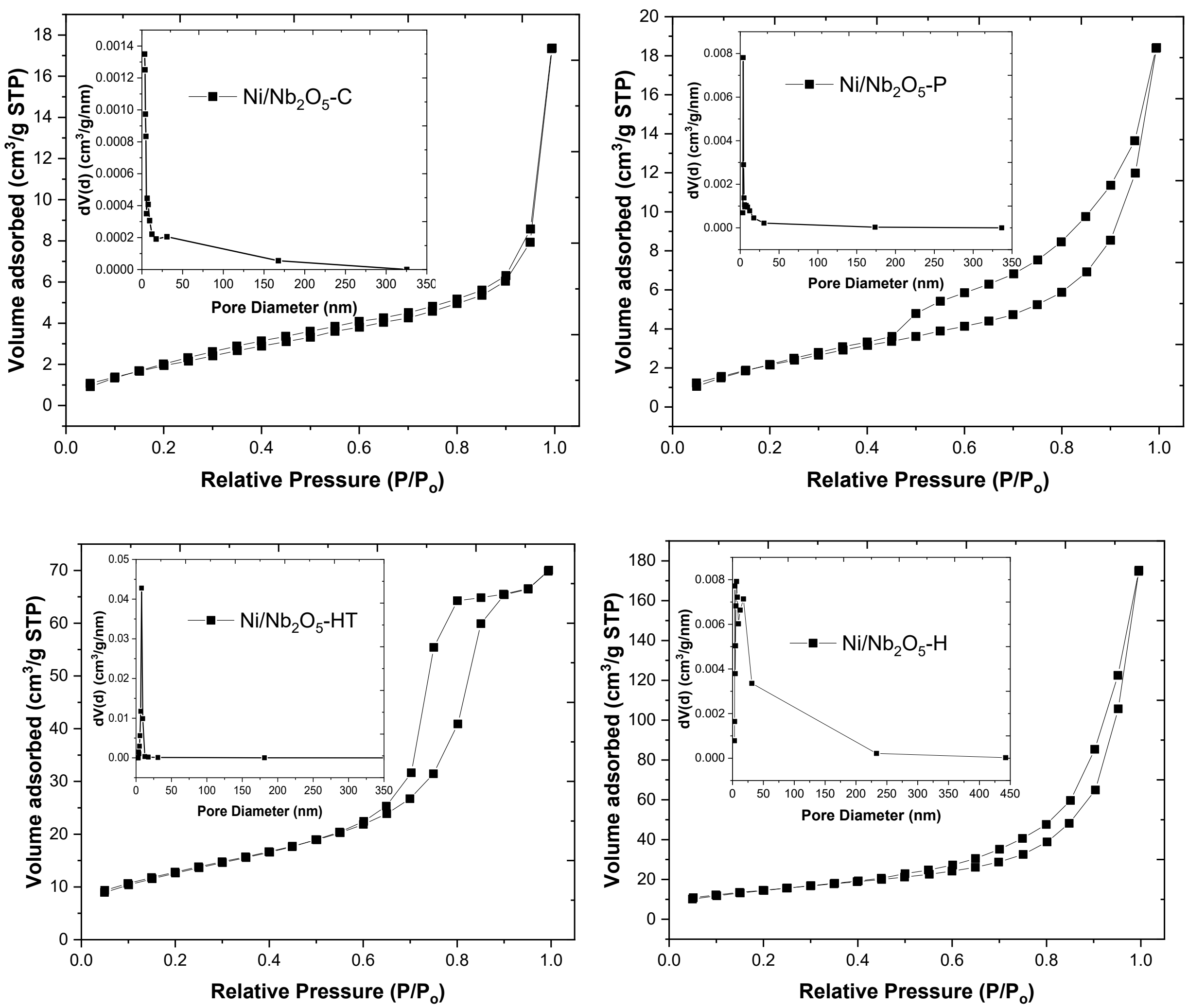

Figure S1. Physisorption isotherm of various Ni/Nb_2O_5 catalysts

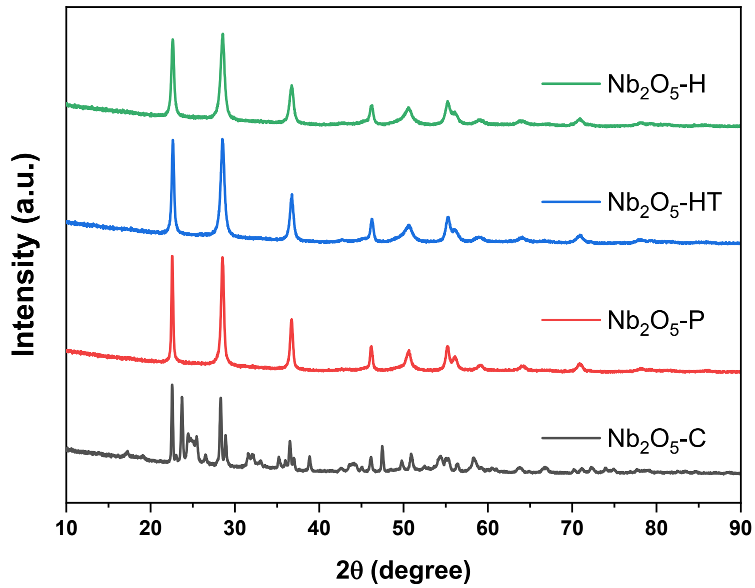

Figure S2. XRD patterns of Nb_2O_5 support

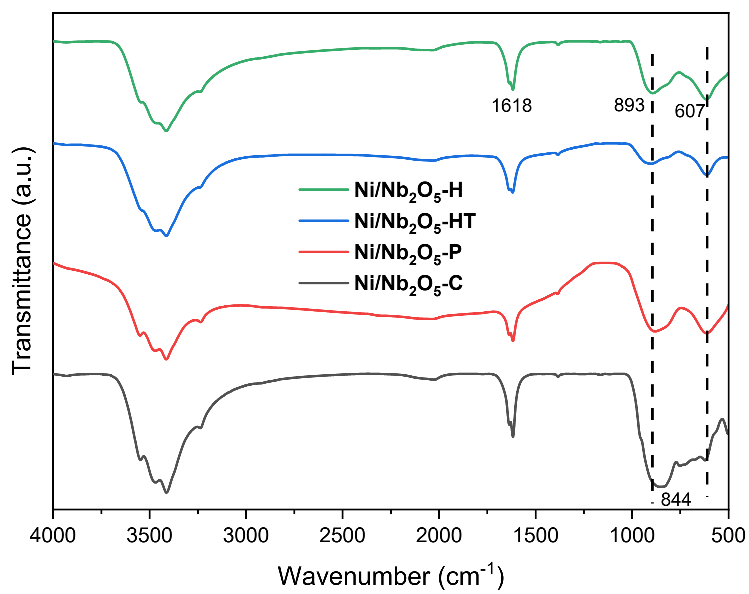

Figure S3. FTIR spectra of Ni/Nb_2O_5 catalysts

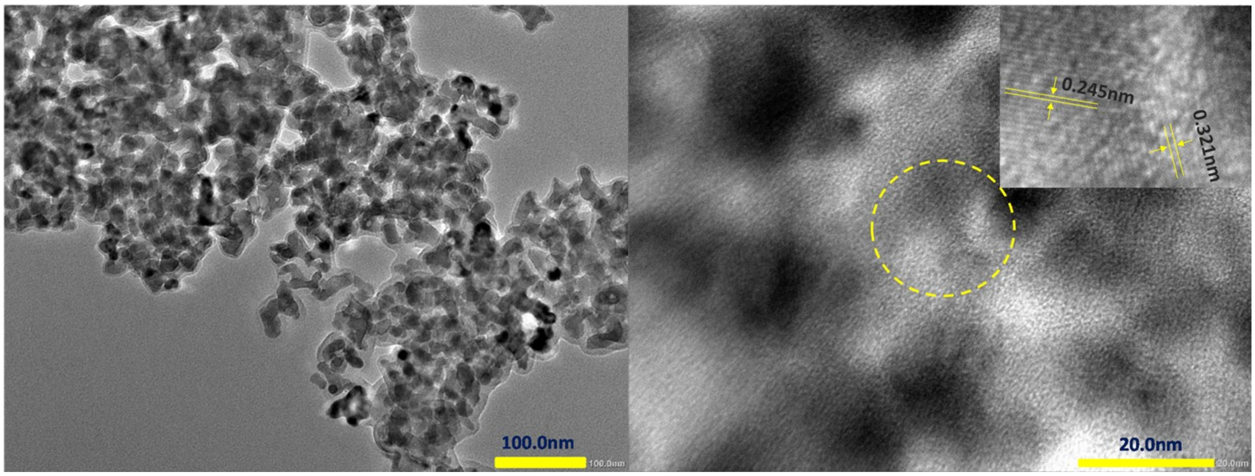

Figure S4. TEM (left) and HR-TEM (right) images of Ni/Nb_2O_5-H catalyst

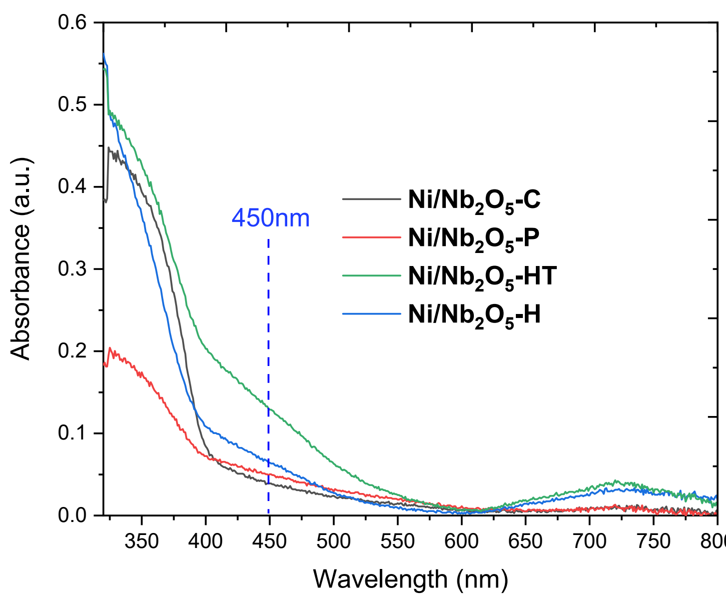

Figure S5. DRS-UV-Vis absorbance spectra of Ni/Nb_2O_5 catalysts

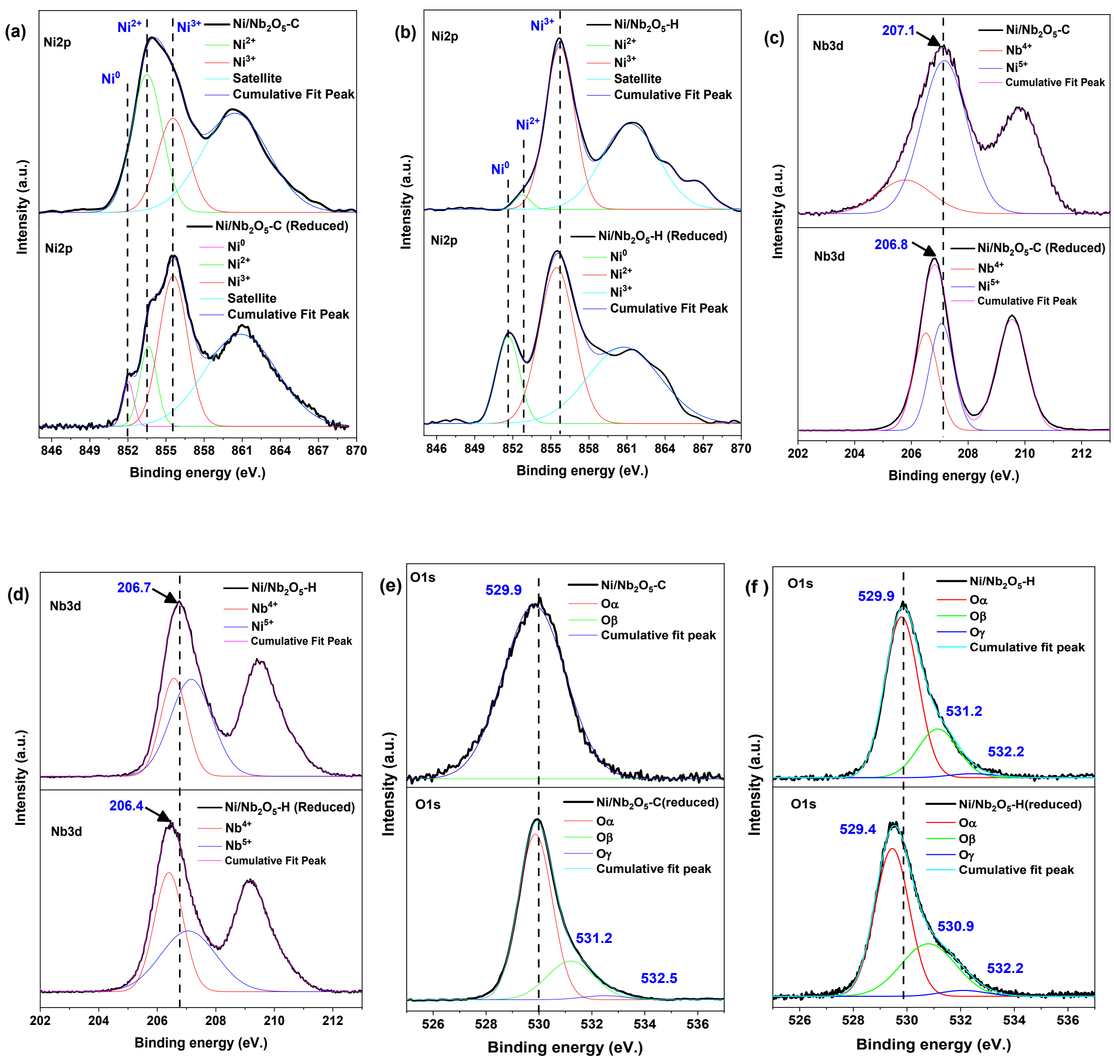

Figure S6. XPS spectra of (a) and (b) for Ni2p, (c) and (d) for Nb3d, (e) and (f) for O1s of Ni/Nb_2O_5-C and Ni/Nb_2O_5-H before and after reduction

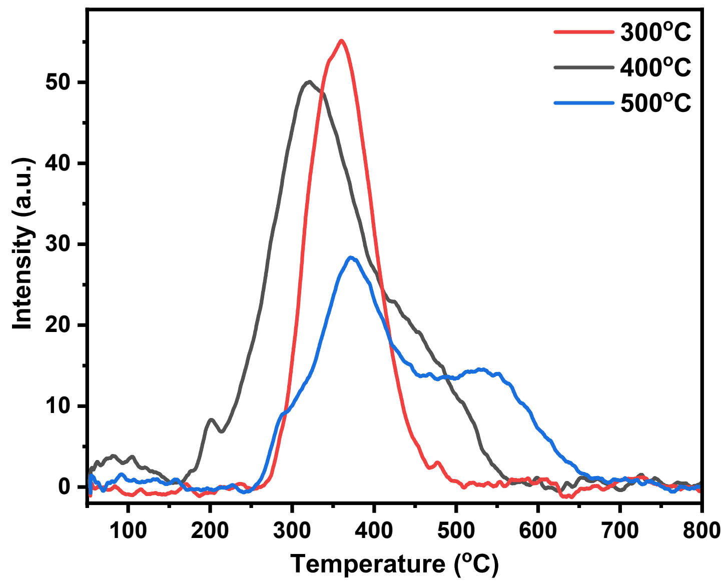

Figure S7. H_2-TPD of Ni/Nb_2O_5-H catalysts at a different reduction temperature

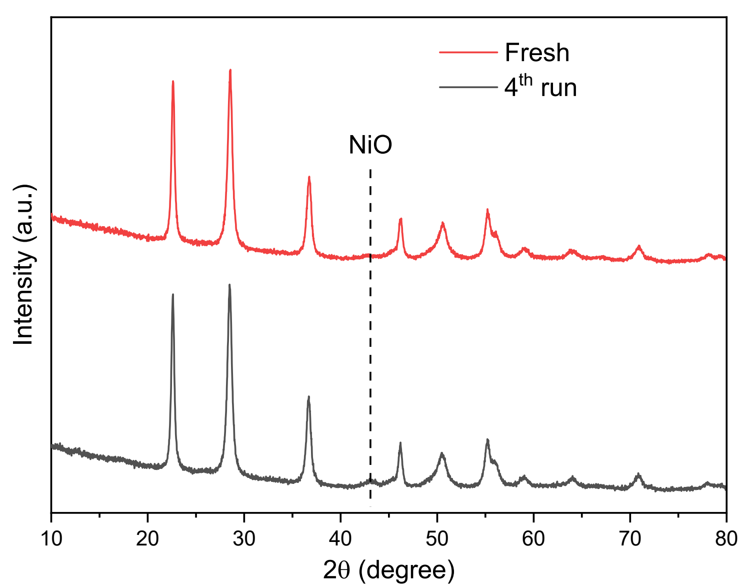

Figure S8. XRD pattern of fresh and spent Ni/Nb_2O_5-H

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