Ligand Tailoring Metal-Support Interactions toward Highly Dispersed Ni/Beta Catalysts for n-Hexane Hydroisomerization

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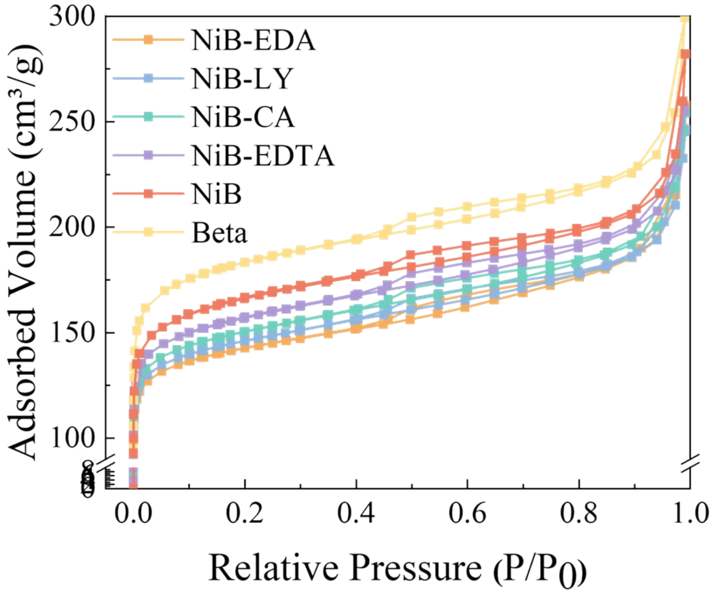

Figure S1. N_2-adsorption and desorption curves for NiB-EDA, NiB-LY, NiB-CA, NiB-EDTA, NiB and Beta catalysts.

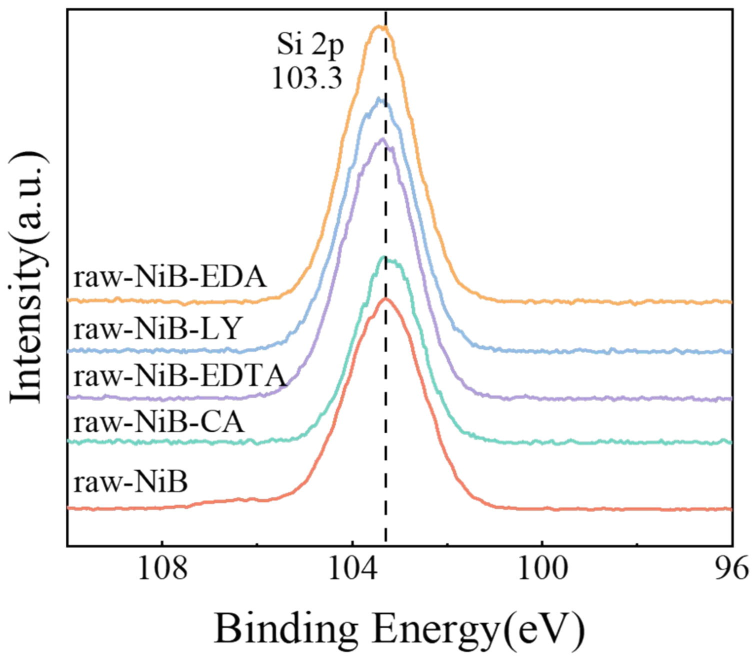

Figure S2. XPS Si 2p spectra of raw-NiB-EDA, raw-NiB-LY, raw-NiB-CA, raw-NiB-EDTA and raw-NiB without calcination.

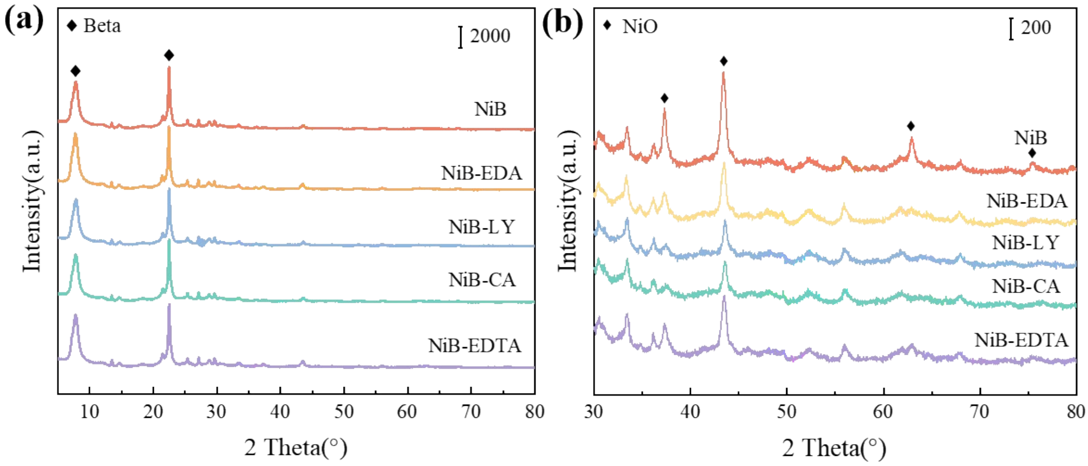

Figure S3. XRD patterns at (a) 4-80°, (b) 30-80° of NiB, NiB-EDA, NiB-LY, NiB-CA and NiB-EDTA.

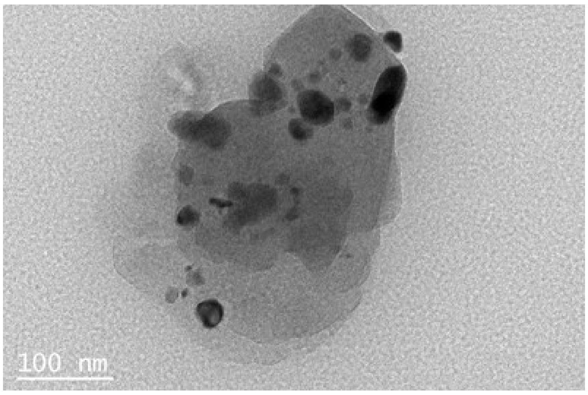

Figure S4. TEM images of NiB catalysts after reduction.

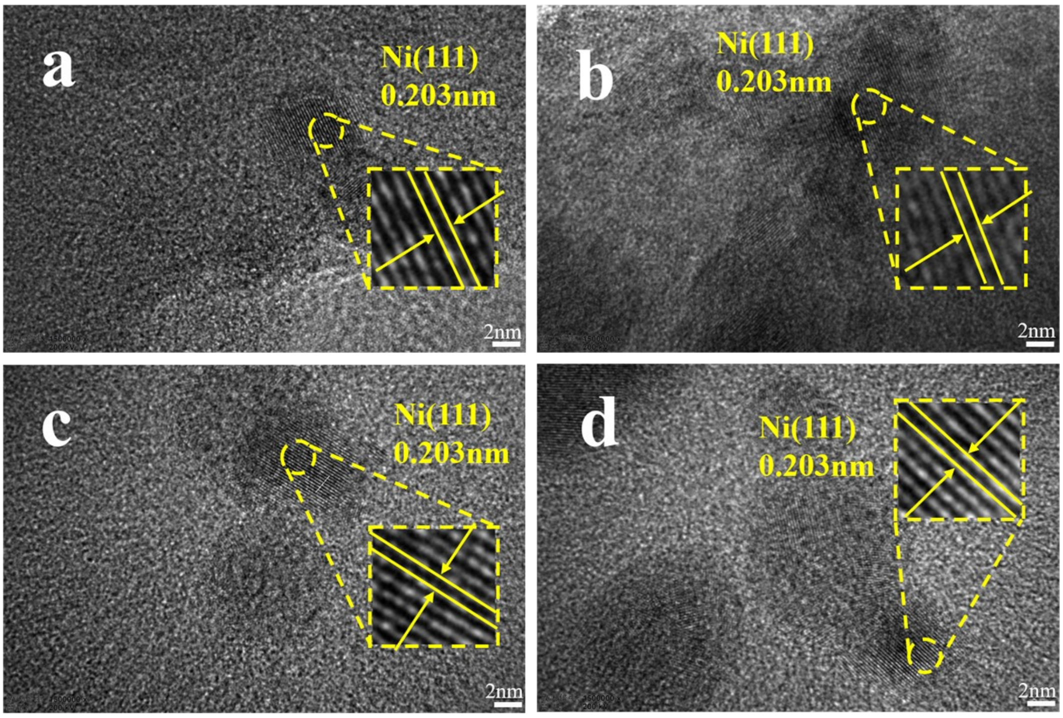

Figure S5. TEM images of NiB-EDA, NiB-LY, NiB-CA and NiB-EDTA catalysts.

The inset is the lattice fringe analysis of the Ni clusters.

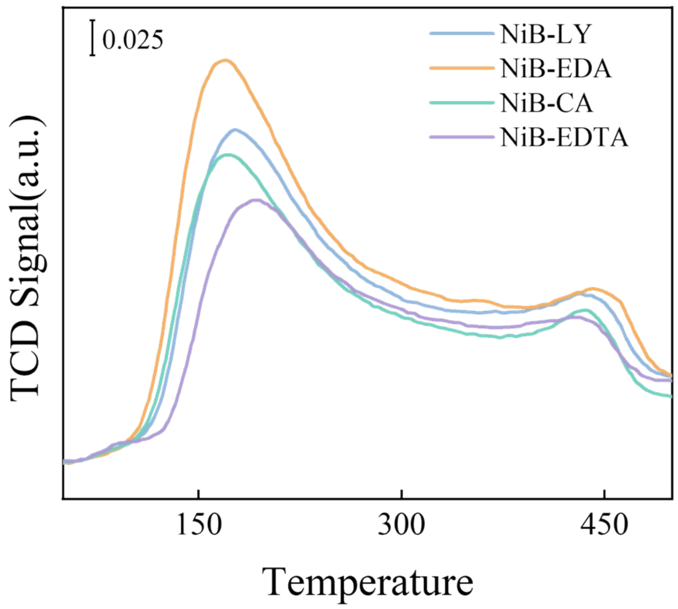

Figure S6. H_2-TPD curves of NiB-EDA, NiB-LY, NiB-CA and NiB-EDTA catalysts.

Table S1. Pore structure features of NiB-EDA, NiB-LY, NiB-CA, NiB-EDTA, NiB and Beta catalysts

Catalyst	S_{BET} (m^2/g)	S_{micro} (m^2/g)	S_{ext} (m^2/g)	V_{tol} (cm^3/g)	V_{micro} (cm^3/g)
NiB-EDA	560.3	439.6	120.7	0.374	0.173
NiB-LY	547.5	452.4	95.1	0.389	0.181
NiB-CA	576.2	451.7	124.5	0.385	0.178
NiB-EDTA	600.3	506.4	93.9	0.396	0.206
NiB	633.5	529.9	103.6	0.426	0.214
Beta	727.2	613.0	114.2	0.464	0.247

Table S2. Elemental analysis of the NiB-EDA, NiB-LY, NiB-CA and NiB-EDTA

Samples	NiB-EDA	NiB-LY	NiB-CA	NiB-EDTA
Si (wt %)	41.5	41.4	41.3	41.7
Al (wt %)	2.3	2.4	2.4	2.2
Ni (wt %)	5.9	6.1	6.2	5.8

Table S3. Isomers performance of catalysts in this work and reference

Samples	Conversion (%)	Isomers yield (%)	Isomers selectivity (%)	Reaction temperature (°C)	Reference
NiB-EDA	81.1	77.2	95.1	280	This work
NiB-Ly	80.5	76.7	95.2	290	This work
NiB-CA	79.4	73.5	92.6	290	This work
NiB-EDTA	77.5	74.0	95.4	290	This work
NiB	75.0	71.3	95.1	290	This work
Ni/SAPO-11	71.6	66.5	92.9	340	[1]
Pt/Ba-ZSM-5	47.8	43.7	91.5	325	[2]
Pt/Sr-MOR	51.3	40.6	79.1	325	[2]
Ni/SAPO-5	77.1	54.0	70.0	360	[3]
Pb/ZSM-22	83.9	76.3	90.9	320	[4]
Pt/HY	80.0	25.0	31.3	300	[5]
NiPB/HB	80.0	78.3	97.9	300	[6]
Ni/SAPO-11	74.3	49.6	66.8	360	[7]
Zn/KCC-1	69.8	67.0	96.0	260	[8]
Commercial Pt based catalysts	83.5	80.3	96.2	-	-

Reference

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