Electronic Supplementary Information (ESI) for:

Rational Design of Ni-based Catalysts derived from Hydrotalcite for Selective Hydrogenation of 5-Hydroxymethylfurfural

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1 Chemicals

The following materials have been used for the preparation of catalysts: nickel(II) nitrate hexahydrate, aluminum(III) nitrate nonahydrate, sodium carbonate and sodium hydroxide. All these chemicals were purchased from Sinopharm. Co. Ltd., and used without further purification. 5-hydroxymethylfurfural was purchased from Shanghai De-Mo Pharmaceutical Science and Technology Limited Company.

2 Characterizations

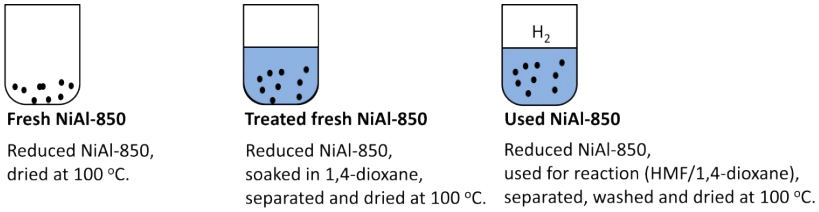
For TPR experiments, 20 mg catalyst was loaded into a quartz tube and heated in 30 mL/min of 10 vol. % H_2/N_2 at a rate of 10 ^oC/min.

For H_2-TPD experiments, the catalysts (200 mg) were first reduced at 500 ^oC for 2 h. The catalysts were then purged with N_2 to remove the physisorbed H_2 at 50 ^oC for 1 h until the baseline was smoothing. Subsequently, the catalysts were heated to 750 ^oC with a rate of 10 ^oC/min.

For CO-TPD experiments, the catalysts (200 mg) were first reduced at 500 ^oC for 2 h. The catalysts were then adsorbed with CO for 0.5 h. Subsequently, the catalysts were heated to 600 ^oC with a rate of 10 ^oC/min.

For NH_3-TPD experiments, the catalysts (200 mg) were pretreated in He at 300 ^oC to remove the adsorbed species for 1 h. After cooling to the room temperature, the catalysts were reduced at 500 ^oC for 2 h, and cooling to room temperature again. After that the catalysts were saturated with NH_3 and then purged with He to remove the physisorbed NH_3 at 100 ^oC for 30 min. Subsequently, the catalysts were heated to 600 ^oC with a rate of 10 ^oC/min.

3 Results and discussion



Scheme S1 Illustrations of used NiAl-850 and reference NiAl-850 catalysts for stability tests and characterizations.

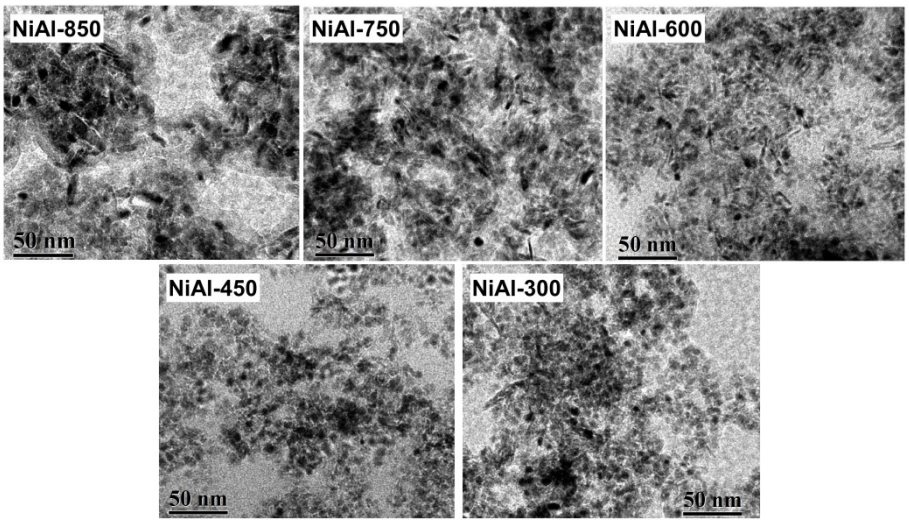


Figure S1 TEM results of reduced NiAl-CT catalyst.

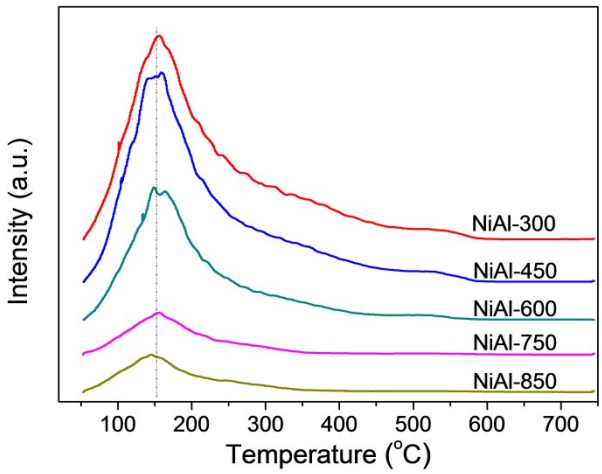


Figure S2 H_2-TPD results of NiAl-CT catalysts.

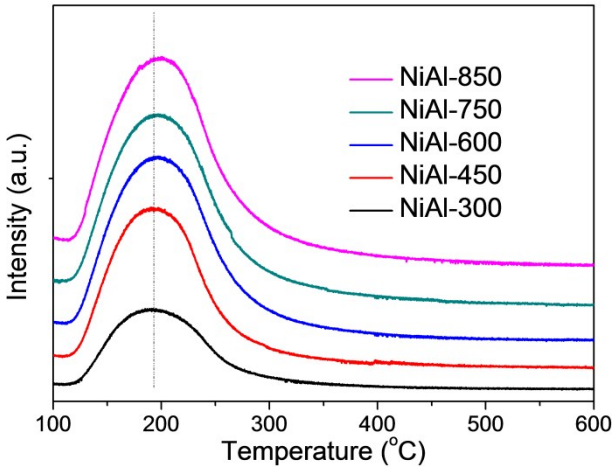


Figure S3 NH_3-TPD results of NiAl-CT catalysts.

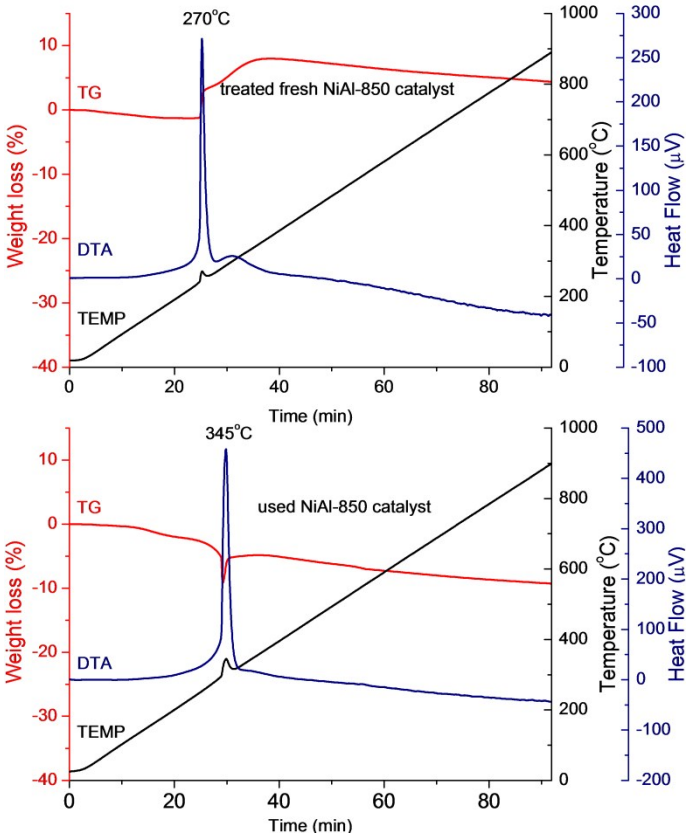


Figure S4 TG results of treated fresh and used NiAl-850 catalyst

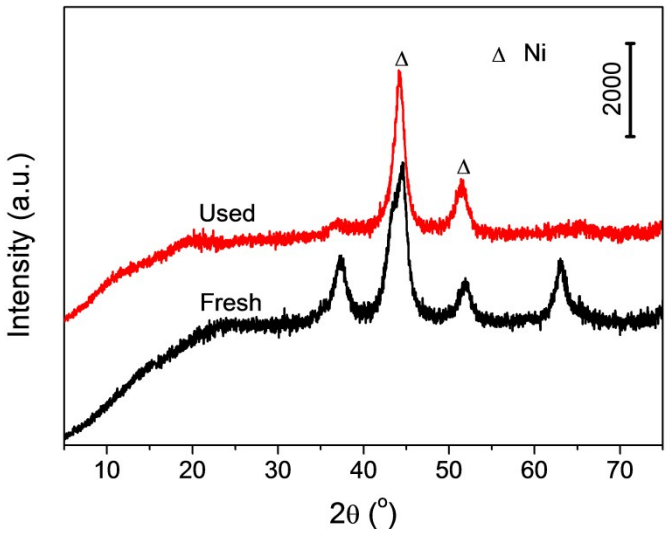
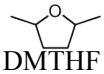
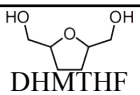
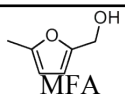


Figure S5 XRD results of treated fresh NiAl-850 and used NiAl-850 catalyst.

Table S1 Hydrogenation of HMF over NiAl-CT catalysts at similar conversions.[a]

Catalyst	t /min	Conv. %	Sel. /%				
			 DMTHF	 DMF	 DHMTHF	 MFA	 DHMF
NiAl-850	90	63.0	0.6	12.9	0	10.7	59.7
NiAl-750	75	55.4	1.4	16.2	1.1	11.0	55.0
NiAl-600	60	50.0	2.4	25.9	0	11.2	45.8
NiAl-450	60	58.0	4.3	32.7	1.3	10.7	36.1
NiAl-300	60	62.9	2.9	26.3	0	10.3	45.6

[a] Reaction conditions: 1.2 MPa, 180 ^{o}C, HMF 1.5 g, 1,4-dioxane 35 ml, catalyst 0.05 g.