Electronic Supplementary Material (ESI) for Reaction Chemistry & Engineering.

Selective hydrogenation of 5-hydroxymethylfurfural to 2,5-bis(hydroxymethyl)furan over Ni–Ga intermetallic catalysts and its kinetic studies

Weixiao Sun†, Fuzeyu Zhong†, Xiaohu Ge*, Wenyao Chen, Gang Qian, Yueqiang Cao, Xuezhi Duan, Xinggui Zhou, Jing Zhang*

State Key Laboratory of Chemical Engineering, School of Chemical Engineering, East China University of Science and Technology; Shanghai, 200237, China.

†These authors contributed equally to this work.

*Corresponding author email: xhge@mail.ecust.edu.cn, jingzhang8507@ecust.edu.cn

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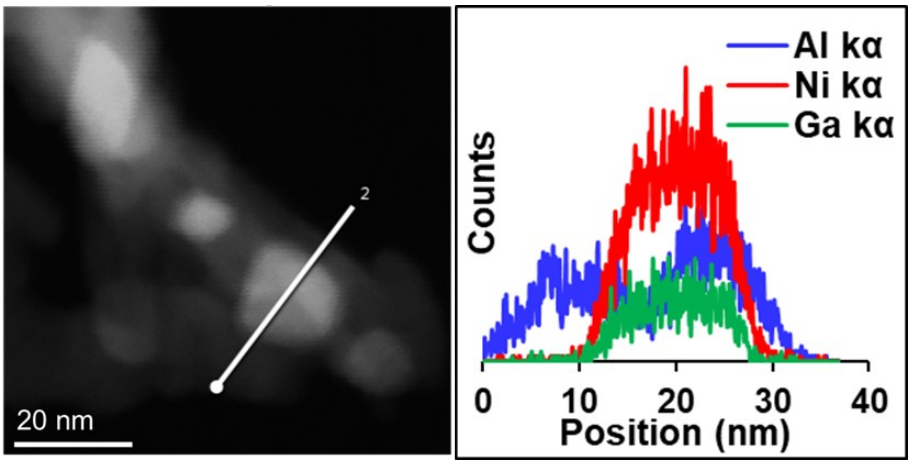
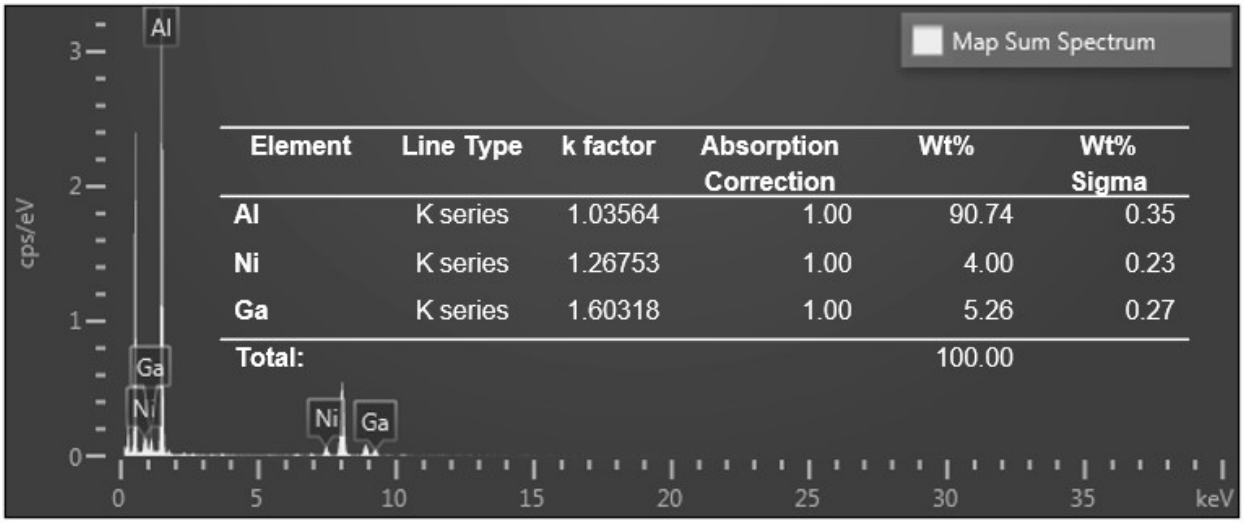


Fig. S1. EDX line scan of the Ni_1Ga_1 intermetallic catalyst.



Element	Line Type	k factor	Absorption Correction	Wt%	Wt% Sigma
Al	K series	1.03564	1.00	90.74	0.35
Ni	K series	1.26753	1.00	4.00	0.23
Ga	K series	1.60318	1.00	5.26	0.27
Total:				100.00	

Fig. S2. The EDX spectra of the Ni_1Ga_1 intermetallic catalyst and total distribution map spectrum.

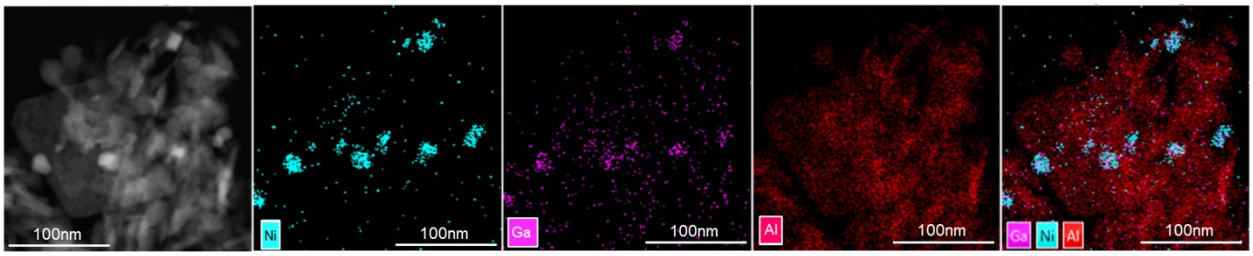


Fig. S3. EDS elemental mapping of the Ni_1Ga_1 intermetallic catalyst.

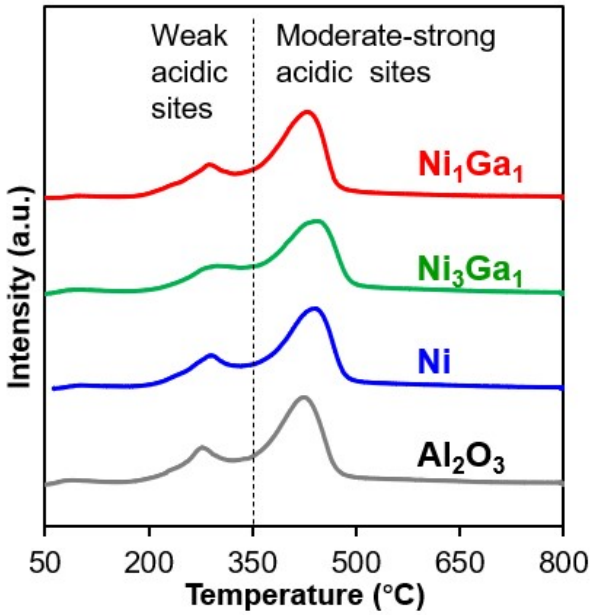


Fig. S4. NH_3-TPD profiles of the referred Ni, Ni_3Ga_1, and Ni_1Ga_1 catalysts.

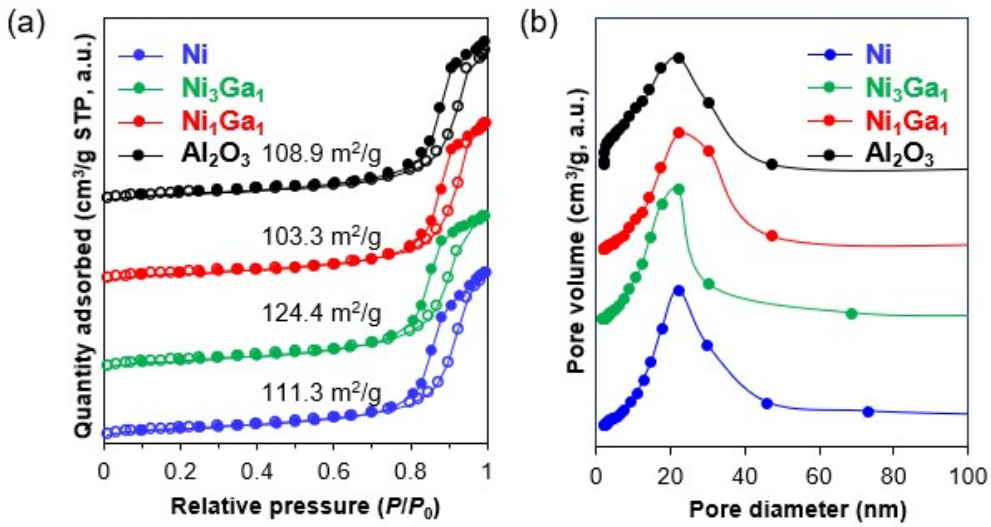


Fig. S5. (a) N_2 adsorption-desorption isotherms and (b) pore size distributions of the referred Ni, Ni_3Ga_1, Ni_1Ga_1 intermetallic catalysts and Al_2O_3 support.

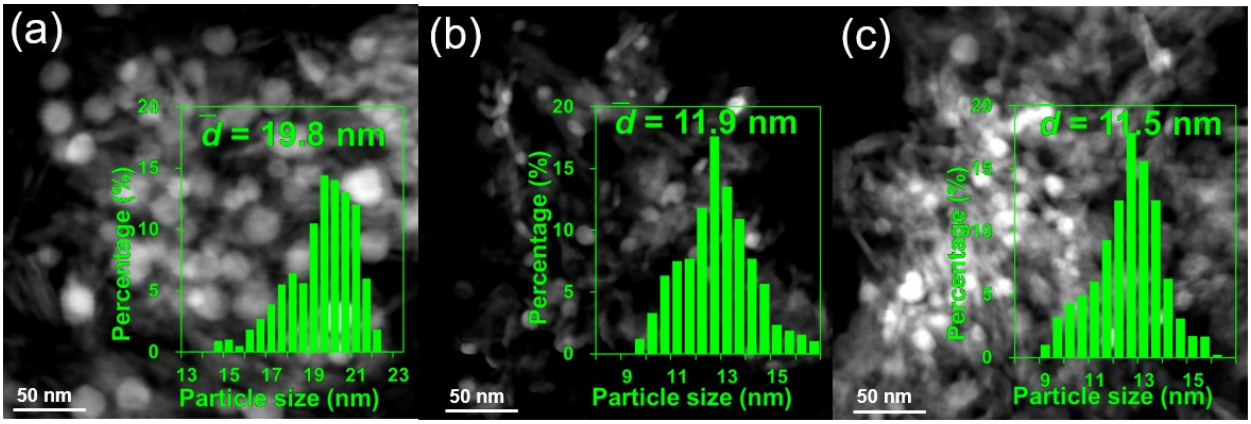


Fig. S6. HAADF-STEM images with corresponding particle size distribution of the post-reaction (a) referred Ni, (b) Ni_3Ga_1, and (c) Ni_1Ga_1 intermetallic catalysts.

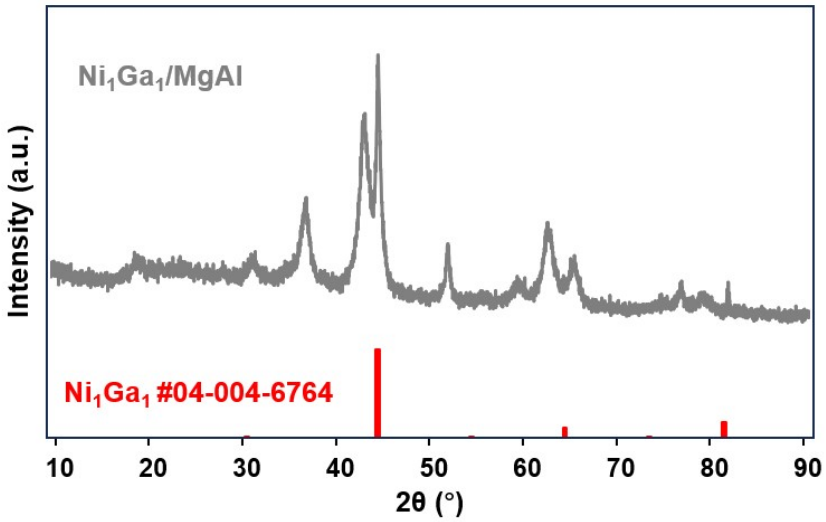


Fig. S7. XRD spectra of the Ni_1Ga_1/MgAl intermetallic catalyst.

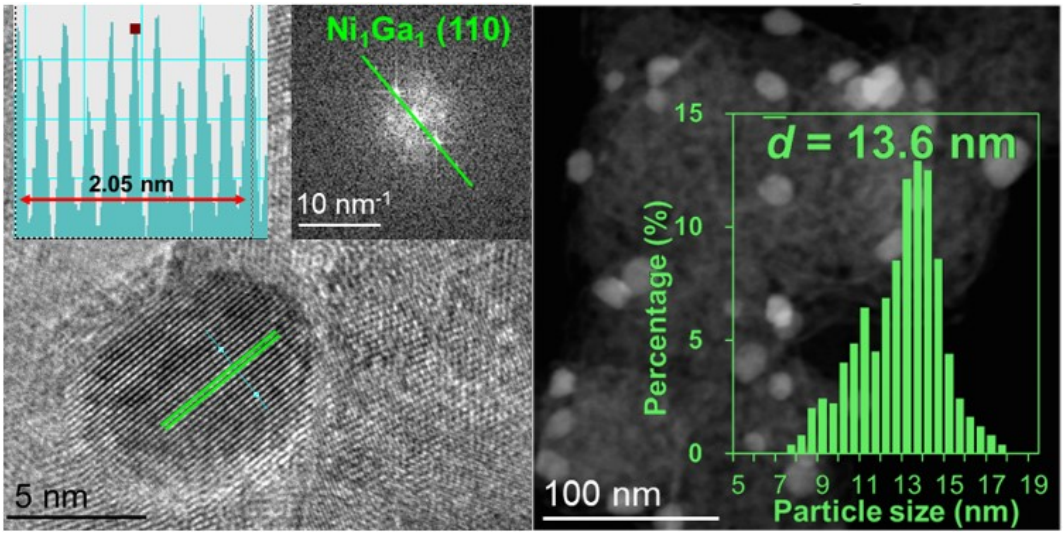


Fig. S8. HRTEM images with lattice fringes and FFT patterns, HAADF-STEM images with corresponding particle size distribution of the Ni_1Ga_1/MgAl intermetallic catalyst.

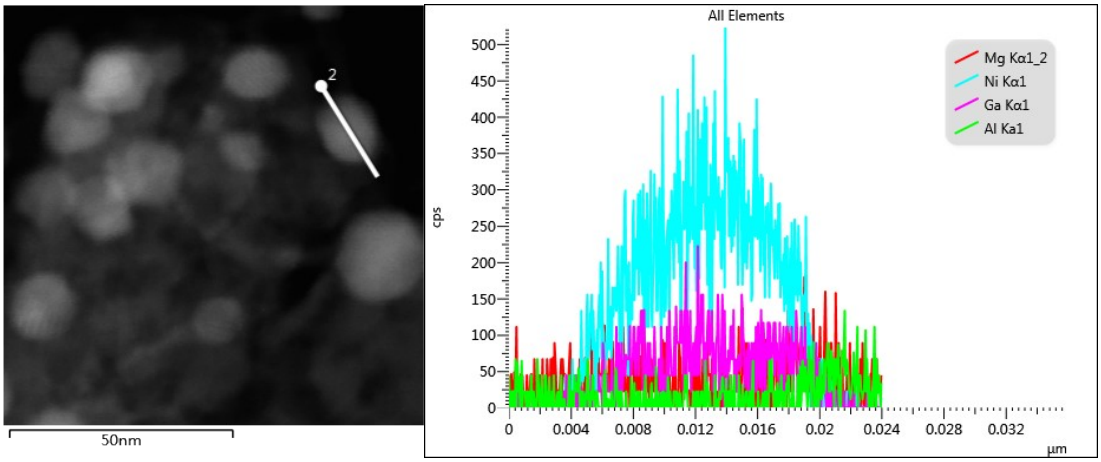


Fig. S9. EDX line scan of the Ni_1Ga_1/MgAl intermetallic catalyst.

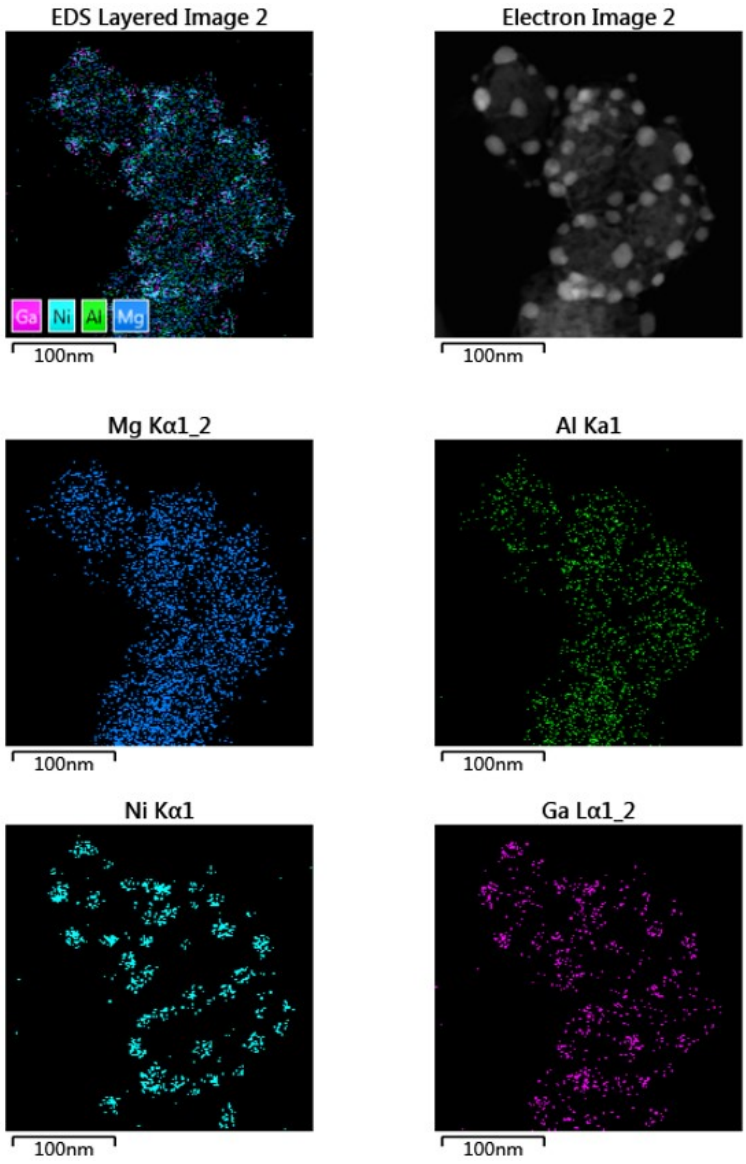


Fig. S10. EDS elemental mapping of the Ni_1Ga_1/MgAl intermetallic catalyst.

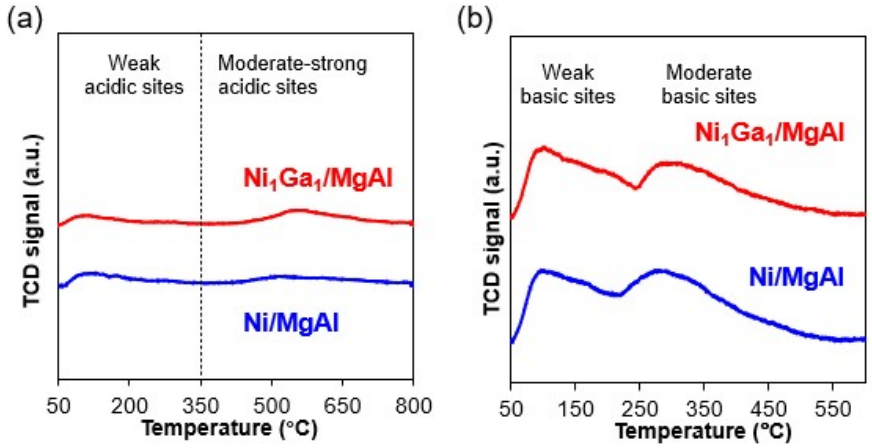


Fig. S11. NH_3-TPD (a) and CO_2-TPD (b) profiles of the referred Ni/MgAl and Ni_1Ga_1/MgAl catalysts.

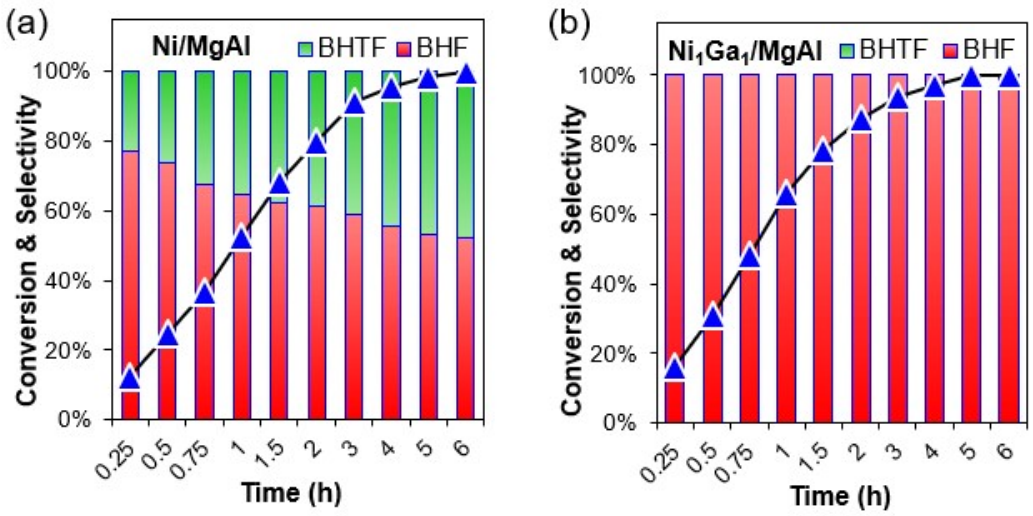


Fig. S12. Conversion of HMF (a) and selectivity of BHF (b) over the referred Ni/MgAl and Ni_1Ga_1/MgAl catalysts (reaction conditions: 20 mL H_2O, 25 mg catalyst, 40 mg HMF, 3.0 MPa H_2, 120 °C).

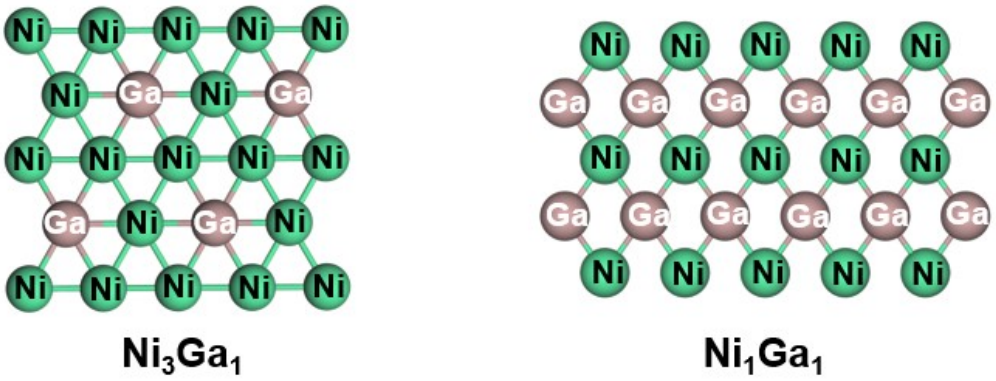


Fig. S13. The Ni atoms coordination environment of Ni_3Ga_1 and Ni_1Ga_1 intermetallics.

Supporting Tables

Table S1. Binding energies & surface compositions (wt.%) of the referred Ni, Ni_3Ga_1, and Ni_1Ga_1 catalysts measured by *in situ* XPS/ICP-MS.

Catalyst	Binding energy (eV)		Fraction (%)		Ni (wt.%)		Ga (wt.%)	
	Ni^0 $2p_{3/2}$	Ga^0 $2p_{3/2}$	$Ni^0/(Ni^0+Ni^{2+})$	$Ga^0/(Ga^0+Ga^{3+})$	XPS	ICP	XPS	ICP
Ni	852.9	/	74.4	/	5.2	5.1	/	/
Ni_3Ga_1	852.7	1116.2	78.0	61.3	6.5	5.0	3.1	1.8
Ni_1Ga_1	852.5	1116.4	81.9	54.4	12.2	5.3	10.6	5.1

Table S2. ICP analysis of the post-reaction solution from the referred Ni, Ni_3Ga_1, and Ni_1Ga_1 intermetallic catalysts after the recyclability test.

Catalyst	Cycle	c_{Ni} (mg/L)
Ni	1	1.85
	2	0.97
	3	0.90
	4	0.88
Ni_3Ga_1	1	0.18
	2	0.10
	3	0.09
	4	0.05
Ni_1Ga_1	1	0.15
	2	0.05
	3	0.08
	4	0.04

Table S3. Catalytic performance of Al_2O_3 catalysts.

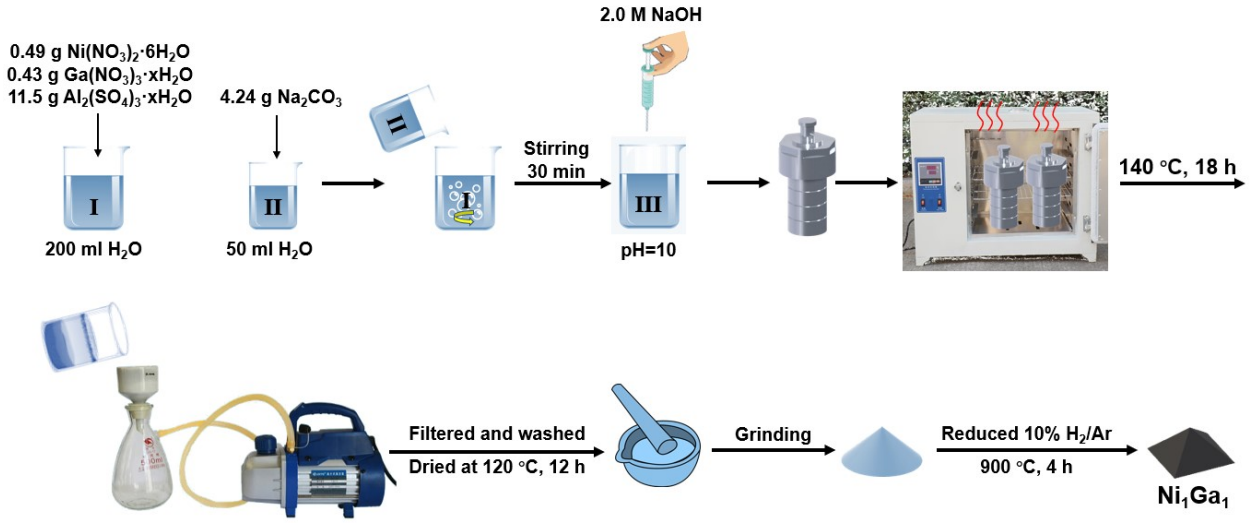
Catalyst	Conv. (%)	Select. BHF (%)	Select. BHTF (%)
Al_2O_3	<0.1	-	-

Table S4. Acidity of intermetallic Ni-Ga over Al_2O_3.

Catalyst	Acidity (mmol/g)
Al_2O_3	1.548
Ni	1.480
Ni_3Ga_1	1.503
Ni_1Ga_1	1.466

Table S5. Acidity and basicity of Ni_1Ga_1/MgAl intermetallic catalysts.

Catalyst	Acidity (mmol/g)	Basicity (mmol/g)
Ni/MgAl	0.114	0.180
Ni_1Ga_1/MgAl	0.142	0.150



Scheme S1. The schematic diagram of Ni_1Ga_1 catalyst preparation.