

Supporting information of

Regulation of Ni/Al₂O₃ catalysts by metal deposition procedures for selective hydrogenation of adiponitrile

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Figure S1. Typical TEM image (a) and HAADF-STEM elemental line scan (b) of Ni/Al₂O₃-NH.

Figure S2. TEM image (a) and HAADF-STEM elemental mappings (b) of Ni/Al₂O₃-U.

Figure S3. Typical TEM and HR-TEM images of Ni/Al₂O₃-U sample.

Figure S4. A typical example of the original deconvolution method of the H₂-TPD curve via the Ni/Al₂O₃-OH catalyst.

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Figure S7. Influences of catalyst amount (a) and ADN/Ni molar ratio (b) on the catalytic performances by Ni/Al₂O₃-OH catalyst. Reaction conditions: 7.0 MPa H₂, 90 °C for 3 h in 25 mL ethanol, 2.5 g ADN for (a) and 500 mg catalyst used for (b).

Figure S8. Circular test of the Ni/Al₂O₃ sample. Reaction conditions: 7.0 MPa H₂, 80 °C for 3 h in 25 mL ethanol, molar ratio of ADN/Ni=13.6.

Figure S9. Typical TEM images of Ni/Al₂O₃-OH sample after reaction.

Figure S10. The external diffusion during the hydrogenation reaction by Ni/Al₂O₃-OH catalyst.

Figure S11. Linear relationship between (a) c_{ADN} and reaction time according to zero-order reaction kinetics, and (b) $\ln c_{ADN}$ and reaction time according to first-order

reaction kinetics by Ni/Al₂O₃-OH over a temperature range of 80-120 °C, 7.0 MPa H₂, 800 rpm for 1.5 h, molar ratio of ADN/Ni=200.

Figure S12. Linear relationship between $\ln r_A$ and $\ln P_{H_2}$ at 90 °C of the ADN hydrogenation by Ni/Al₂O₃-OH

Figure S13. Catalytic performance by Ni/Al₂O₃-OH and Ni/Al₂O₃-U samples. Reaction conditions: 7.0 MPa H₂, 90 °C for 3 h in 25 mL ethanol, molar ratio of ADN/Ni=13.6.

Table S1. The R² for mathematics fitting of kinetic reaction models during the ADN hydrogenation by Ni/Al₂O₃-OH catalysts.^a

Table S2. The reaction rate (r_A) and activation energy (E_a) for the hydrogenation of ADN by different Ni/Al₂O₃ catalysts.^a

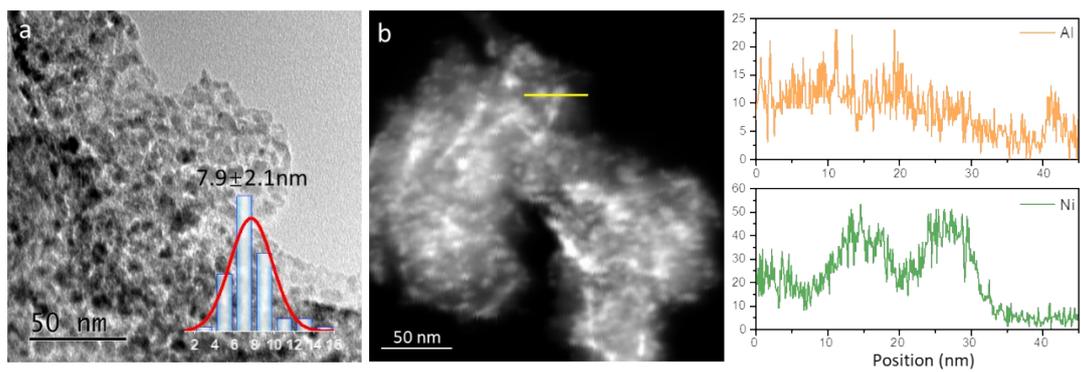


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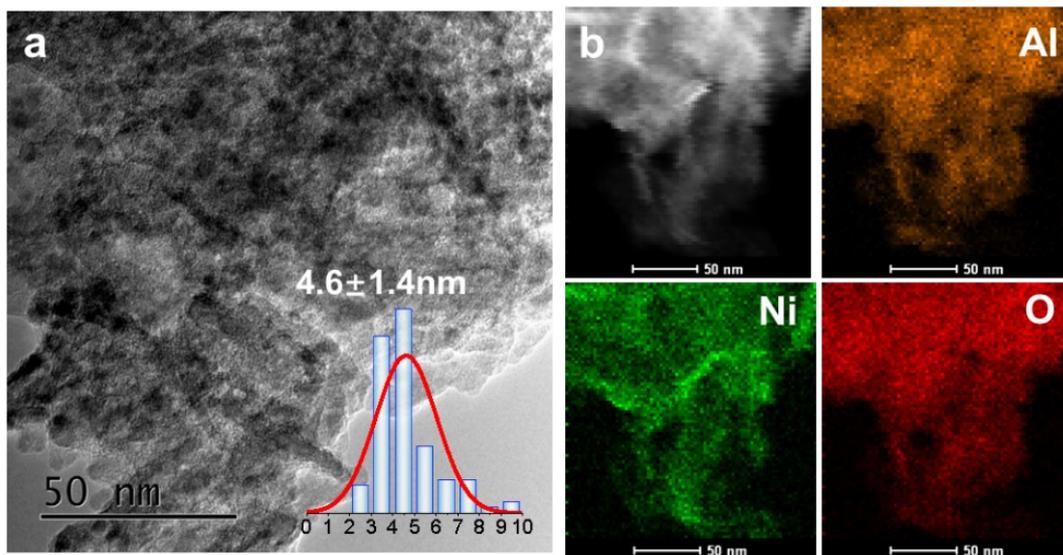


Figure S2. TEM image (a) and HAADF-STEM elemental mappings (b) of Ni/Al₂O₃-U.

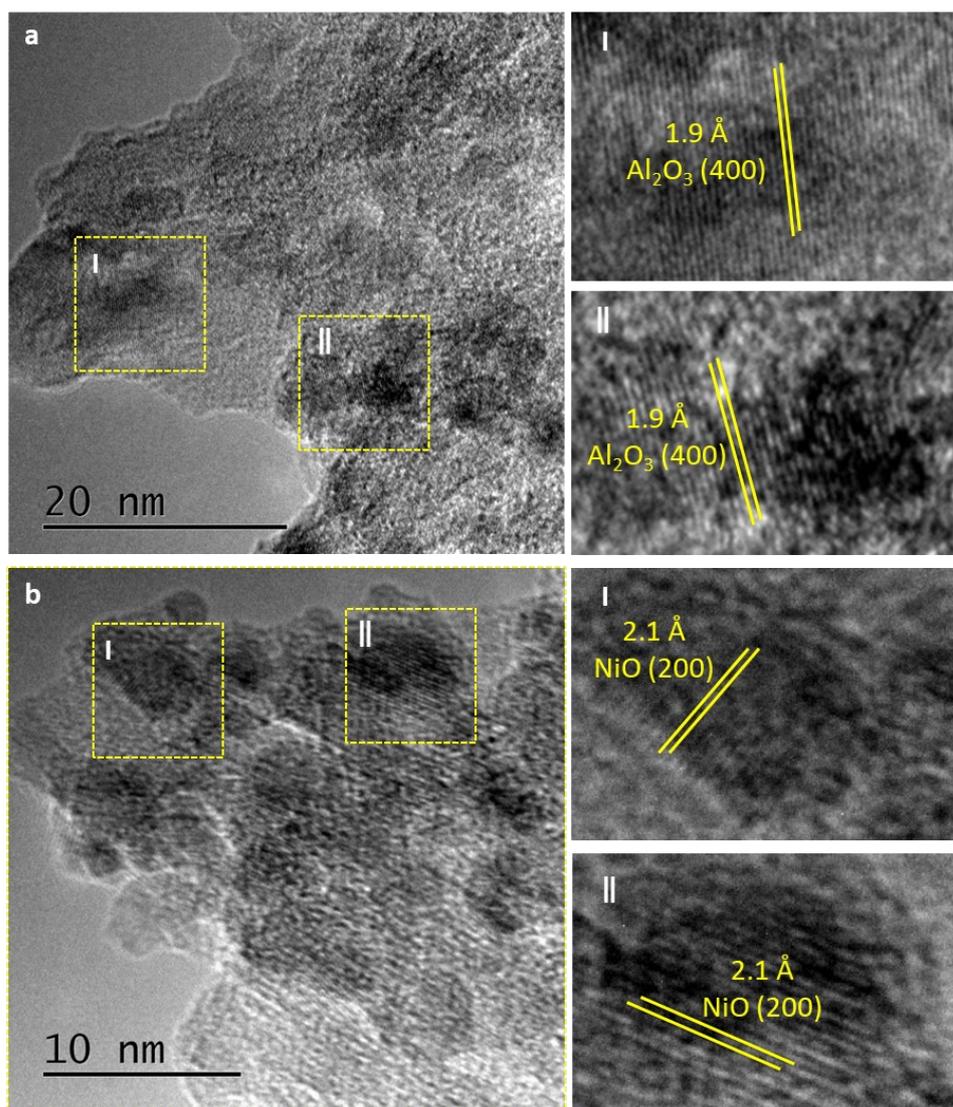


Figure S3. Typical TEM and HR-TEM images of Ni/Al₂O₃-U sample.

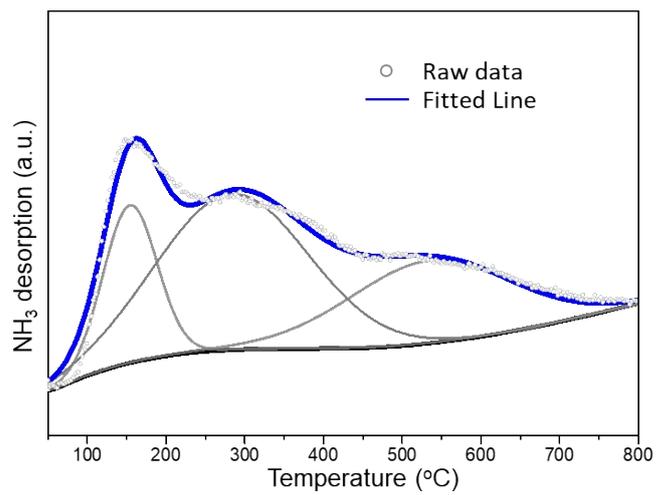


Figure S4. A typical example of the original deconvolution method of the H₂-TPD curve for the Ni/Al₂O₃-OH catalyst.

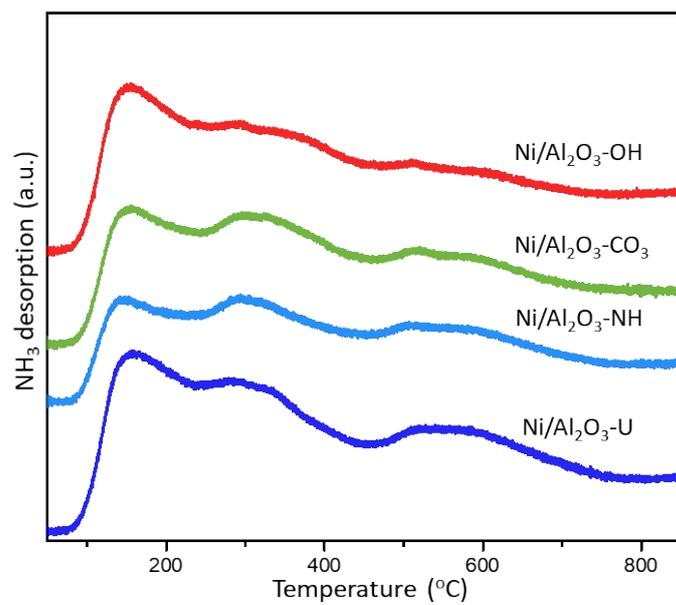


Figure S5. NH₃-TPD curves of different Ni/Al₂O₃ catalysts.

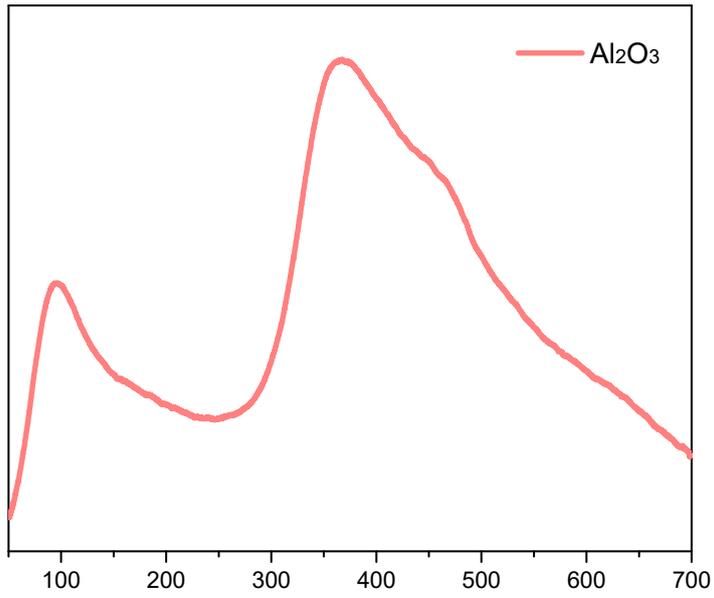


Figure S6. NH₃-TPD curve of Al₂O₃.

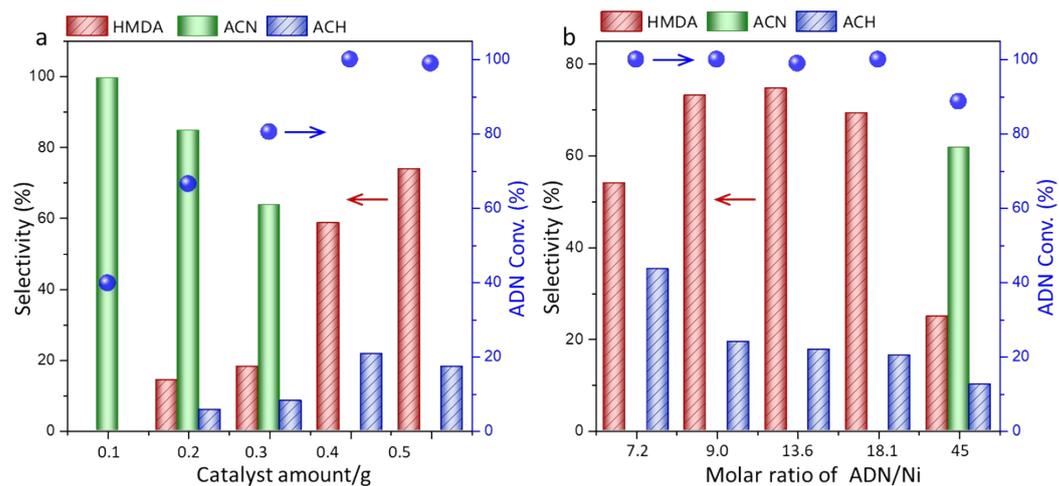


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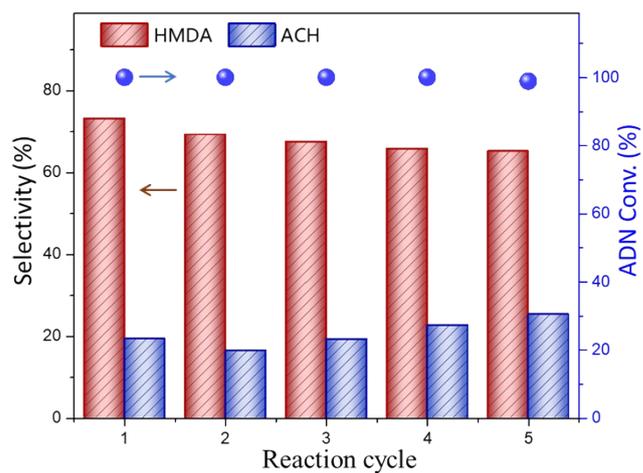


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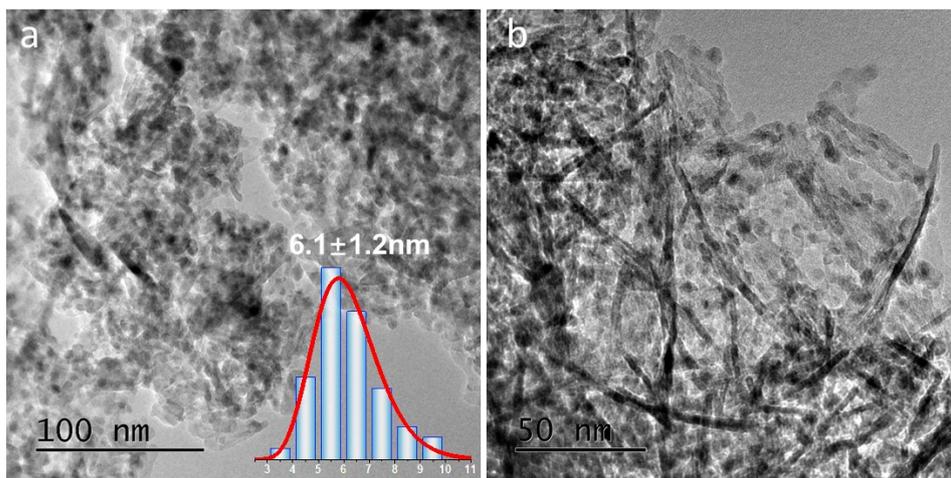


Figure S9. Typical TEM images of Ni/Al₂O₃-OH sample after reaction.

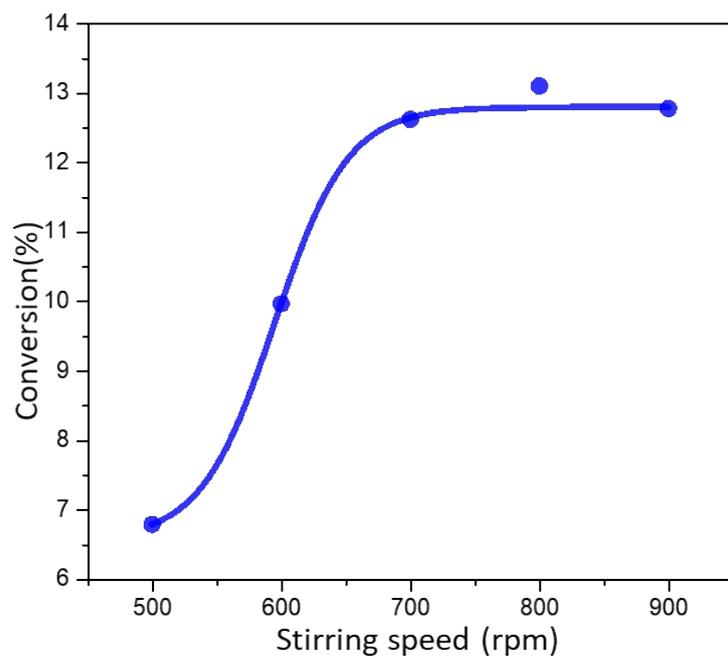


Figure S10. The external diffusion during the hydrogenation reaction by Ni/Al₂O₃-OH catalyst.

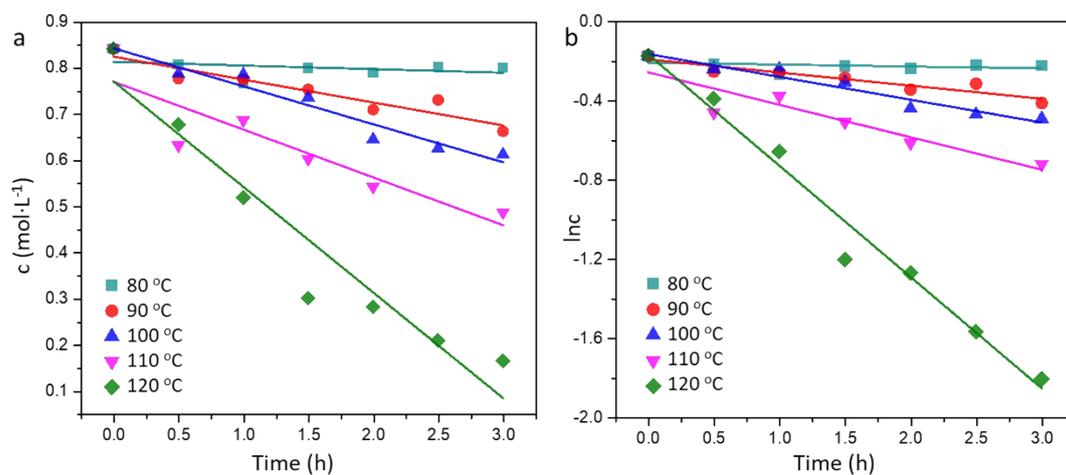


Figure S11. Linear relationship between (a) c_{ADN} and reaction time according to zero-order reaction kinetics, and (b) $\ln c_{\text{ADN}}$ and reaction time according to first-order reaction kinetics by Ni/Al₂O₃-OH over a temperature range of 80-120 °C, 7.0 MPa H₂, 800 rpm for 1.5 h, molar ratio of ADN/Ni=200.

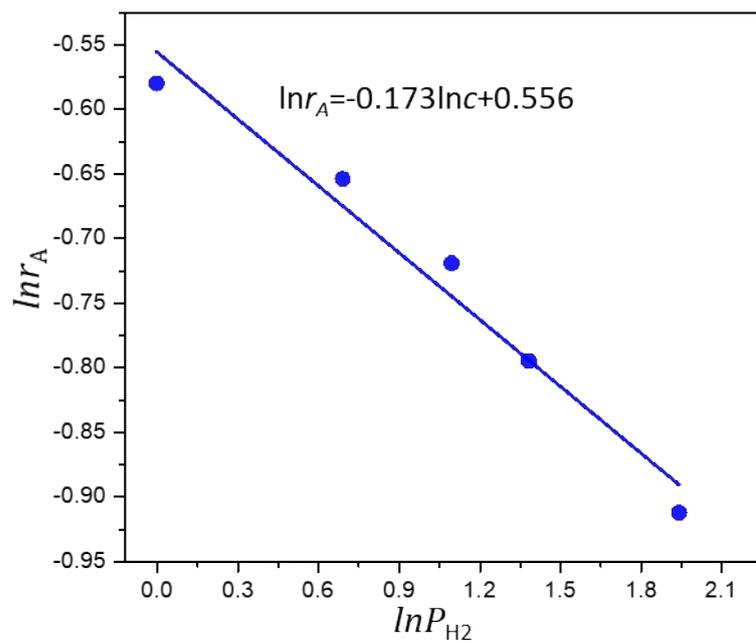


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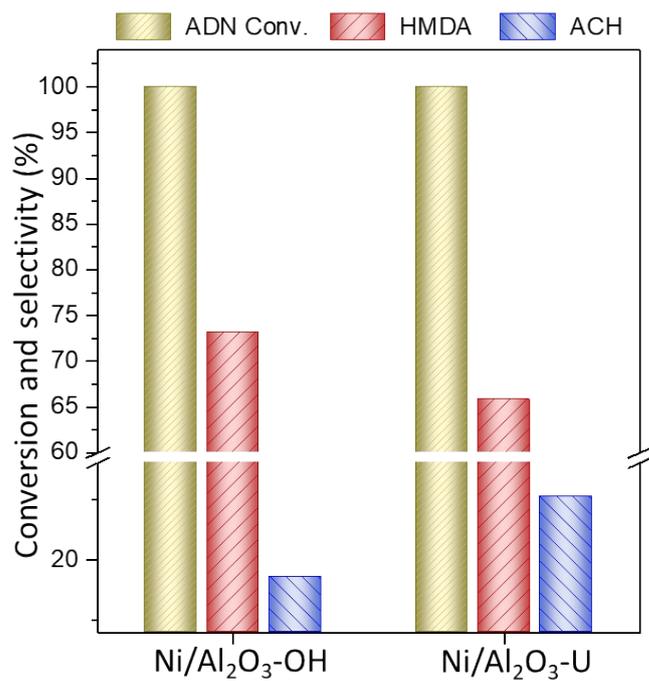


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Table S1. The R^2 for mathematics fitting of kinetic reaction models during the ADN hydrogenation by Ni/Al₂O₃-OH catalysts.^a

Ni/Al ₂ O ₃ -OH catalyst	80 °C	90 °C	100 °C	110 °C	120 °C
Zero-order	0.38	0.94	0.97	0.90	0.96
First-order	0.37	0.94	0.97	0.93	0.99
Second-order	0.73	0.94	0.97	0.95	0.98

^a Experiments carried out over a temperature range of 80-120 °C, 7.0 MPa H₂, 800 rpm for 1.5 h, molar ratio of ADN/Ni=200.

Table S2. The reaction rate (r_A) and activation energy (E_a) for the hydrogenation of ADN by different Ni/Al₂O₃ catalysts.^a

Catalyst	Reaction rate (mol·L ⁻¹ ·h ⁻¹)					E _a (kJ/mol)
	80 °C	90 °C	100 °C	110 °C	120 °C	
Ni/Al ₂ O ₃ -OH	0.047	0.059	0.113	0.160	0.243	49.6
Ni/Al ₂ O ₃ -CO ₃	0.021	-	0.036	0.116	0.164	62.6
Ni/Al ₂ O ₃ -NH	0.019	-	0.077	0.099	0.236	69.4
Ni/Al ₂ O ₃ -U	0.009	0.018	0.041	0.048	0.119	72.0

^a Experiments carried out over a temperature range of 353–393 K, 7.0 MPa H₂, 800 rpm for 1.5 h, molar ratio of ADN/Ni=200.