

Supporting information file for

Structure and surface characteristics of Fe-promoted Ni/Al₂O₃ catalysts for hydrogenation of 1,4-butyne-1,3-diol to 1,4-butanediol in a slurry-bed reactor

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Table S1. Elemental composition of various catalysts.

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Fig. S1 XRD patterns of reduced Ni/Al₂O₃ and Ni-xFe/Al₂O₃ with varied Fe loading (1, 3, 5, 7, 9 wt.%)

Fig. S2 XPS spectra of reduced Fe/Al₂O₃ and Ni-3Fe/Al₂O₃ catalysts.

Fig. S3 (a) HRTEM images, and (b-c) SAED pattern Ni/Al₂O₃. (d-f) STEM image of Ni-3Fe/Al₂O₃ nanoparticles along with its elemental mapping images [Al (purple), Fe (red), Ni (blue) and O (green)].

Fig. S4 HRTEM images of (a) Ni-3Fe/Al₂O₃, (b) Ni/Al₂O₃.

Fig. S5 Effects of Fe content on hydrogenation of BYD to BED.

Fig. S6 Raman spectra of used Ni/Al₂O₃ and Ni-3%Fe/Al₂O₃ catalysts.

Table S1. Elemental composition of various catalysts.

Catalysts	Elemental composition by XRF (weight %)			
	Ni	Fe	Al	O
Ni/Al ₂ O ₃	25.03	/	35.94	39.03
Ni-3%Fe/Al ₂ O ₃	25.26	3.51	33.90	37.37
Ni-5%Fe/Al ₂ O ₃	25.56	5.48	29.83	39.13
20%Fe/Al ₂ O ₃	/	19.60	37.66	42.74

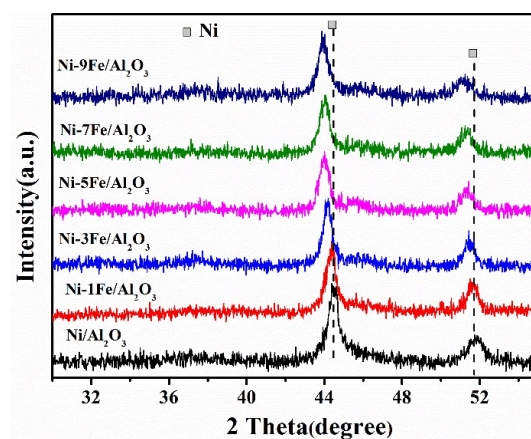


Fig. S1 XRD patterns of reduced Ni/Al₂O₃ and Ni-xFe/Al₂O₃ with varied Fe loading (1, 3, 5, 7, 9 wt.%)

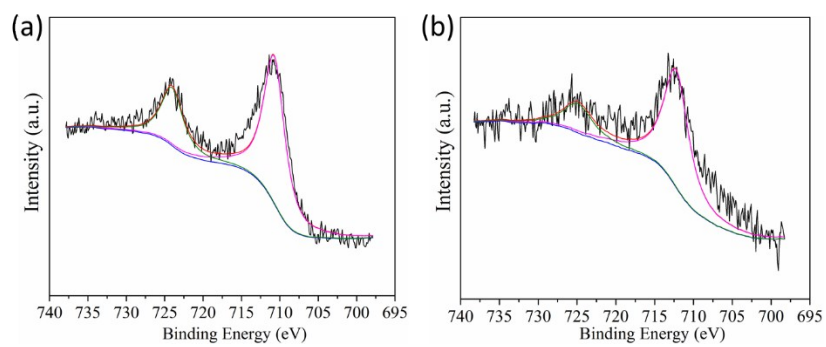


Fig. S2 XPS spectra of reduced Fe/Al₂O₃ and Ni-3Fe/Al₂O₃ catalysts.

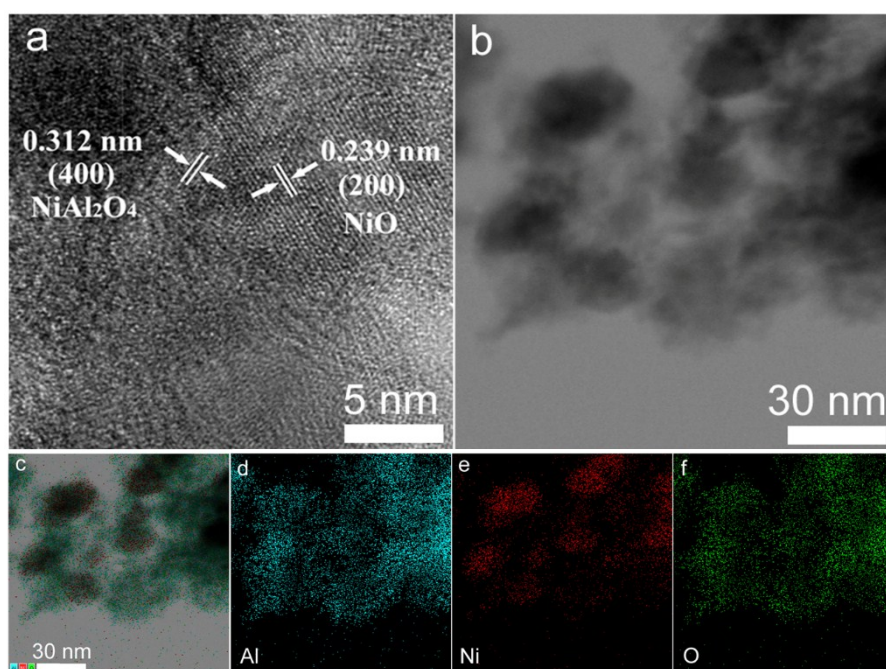


Fig. S3 (a) HRTEM images, and (b-c) SAED pattern $\text{Ni-3Fe/Al}_2\text{O}_3$. (d-f) STEM image of $\text{Ni-3Fe/Al}_2\text{O}_3$ nanoparticles along with its elemental mapping images [Al (purple), Fe (red), Ni (blue) and O (green)].

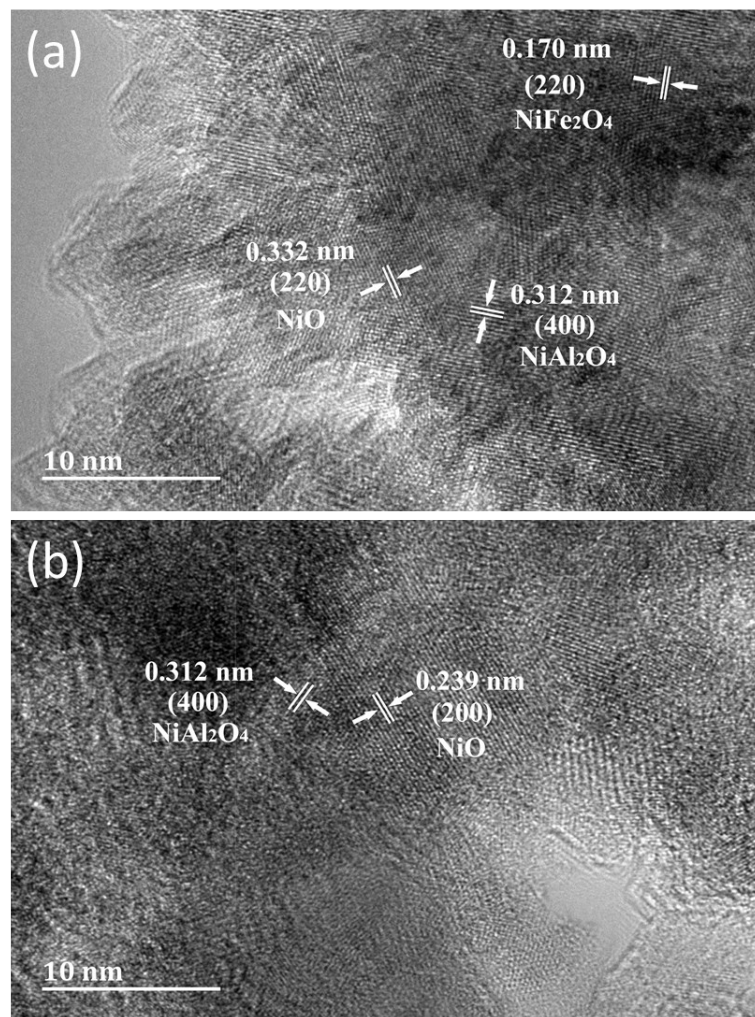


Fig. S4 HRTEM images of (a) $\text{Ni-3Fe}/\text{Al}_2\text{O}_3$, (b) $\text{Ni}/\text{Al}_2\text{O}_3$.

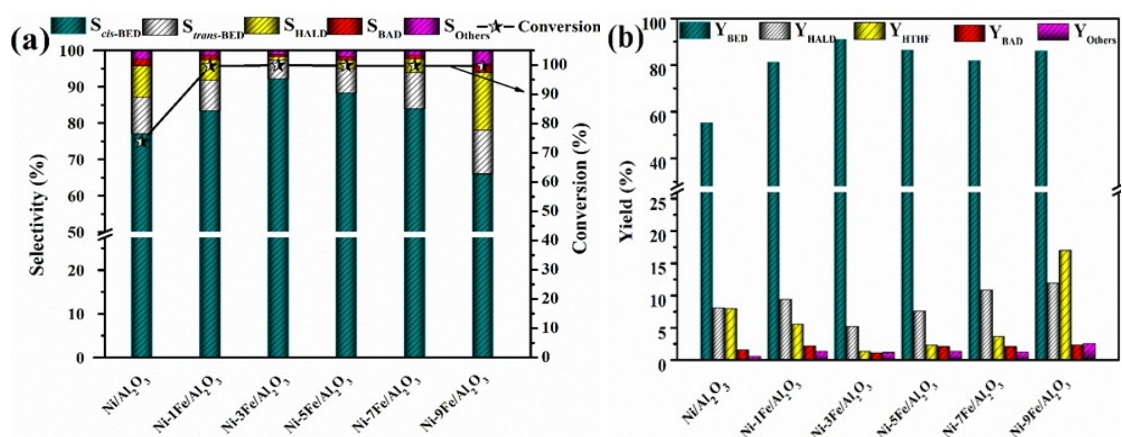


Fig. S5 Effects of Fe content on hydrogenation of BYD to BED

Table S2. Catalytic properties of Ni/Al₂O₃ for the hydrogenation of BYD with different reaction time

Time (min)	C _{BYD} (%)	S _{cis-BED} (%)	S _{trans-BED} (%)	S _{HALD} (%)	S _{BAD} (%)	S _{others} (%)
5	13.8	97.0	1.2	1.5	0.0	0.3
30	50.3	92.8	3.7	2.1	0.5	0.8
60	58.2	87.8	6.3	3.9	0.8	1.1
180	73.8	77.1	10.0	8.7	1.8	2.4

Table S3. Catalytic properties of Ni-3%Fe/Al₂O₃ for the hydrogenation of BYD with different reaction time

Time (min)	C _{BYD} (%)	S _{cis-BED} (%)	S _{trans-BED} (%)	S _{HALD} (%)	S _{BAD} (%)	S _{others} (%)
5	19.3	98.2	0.7	0.8	0.0	0.3
30	80.6	97.7	1.2	0.7	0.0	0.3
60	87.1	95.2	2.6	0.8	0.2	0.2
180	99.9	92.1	5.2	1.0	0.5	1.1

Table S4. Catalytic properties of Ni-5%/Al₂O₃ for the hydrogenation of BYD with different reaction time

Time (min)	C _{BYD} (%)	S _{cis-BED} (%)	S _{trans-BED} (%)	S _{HALD} (%)	S _{BAD} (%)	S _{others} (%)
5	18.4	99.3	0.3	0.2	0.0	0.2
30	82.6	96.8	1.9	0.5	0.2	0.5
60	88.3	94.8	3.4	0.7	0.2	0.8
180	99.8	88.3	6.6	2.4	0.9	1.6

Reaction conditions: 4.0 MPa (pure H₂), 393K, 0.6 g reduced catalysts, 750 rpm, 30 mL 1,4-butyndiol (30 wt.% in water)

Table S5. Catalytic properties of 20%Fe/Al₂O₃ and FeAl₂O₄ catalyst for the hydrogenation of 1,4-butyne-1,3-diol

Catalysts	C _{BYD} (%)	S _{cis-BED} (%)	S _{trans-BED} (%)	S _{HALD} (%)	S _{BAD} (%)	S _{others} (%)
20%Fe/Al ₂ O ₃	0.5	99.8	0.0	0.0	0.0	0.2
FeAl ₂ O ₄	0.8	99.9	0.0	0.0	0.0	0.1

Reaction conditions: 4.0 MPa (pure H₂), 393K, 0.6 g reduced catalysts, 750 rpm, 30 mL 1,4-butyne-1,3-diol (30 wt.% in water)

Table S6. Acid-base properties according to NH₃ and CO₂ TPD data

Catalysts	NH ₃ uptake amount mmol/g	CO ₂ uptake amount mmol/g
Ni/Al ₂ O ₃	15.620	10.558
Ni-3%Fe /Al ₂ O ₃	16.311	10.511
Ni-5%Fe /Al ₂ O ₃	16.235	10.277

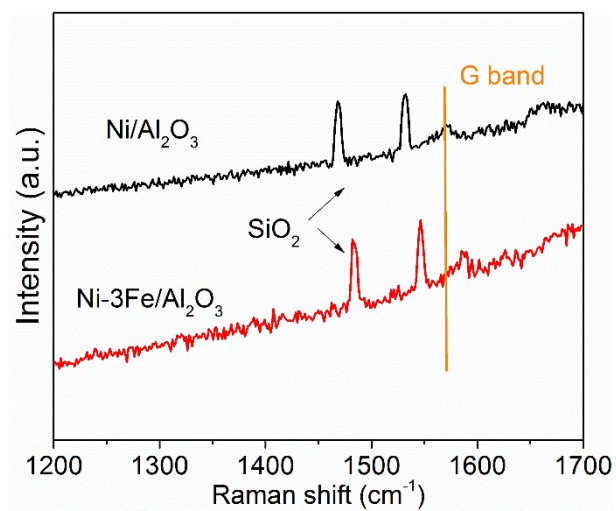


Fig. S6 Raman spectra of used Ni/Al₂O₃ and Ni-3%Fe/Al₂O₃ catalysts