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Supporting Information

Clean hydrogen production from ammonia decomposition over zeolite 13X-supported Ni catalysts

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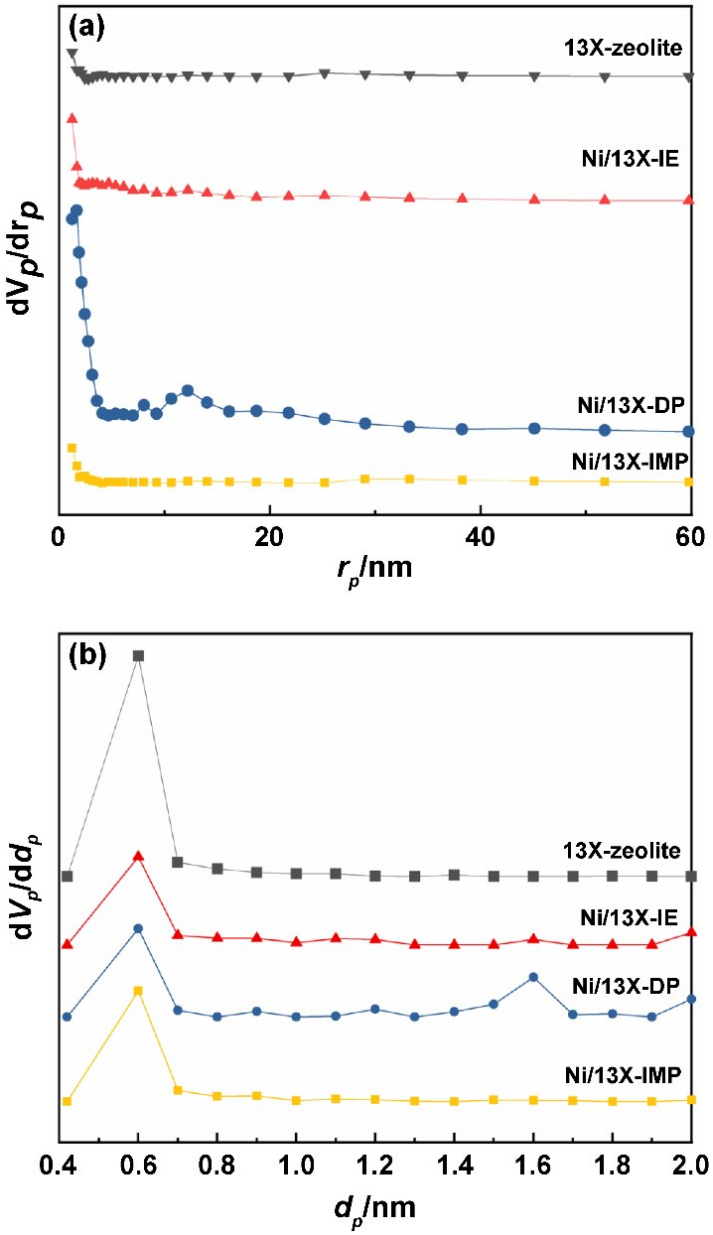

Figure S1. Pore size distribution of Ni/zeolite 13X catalysts.

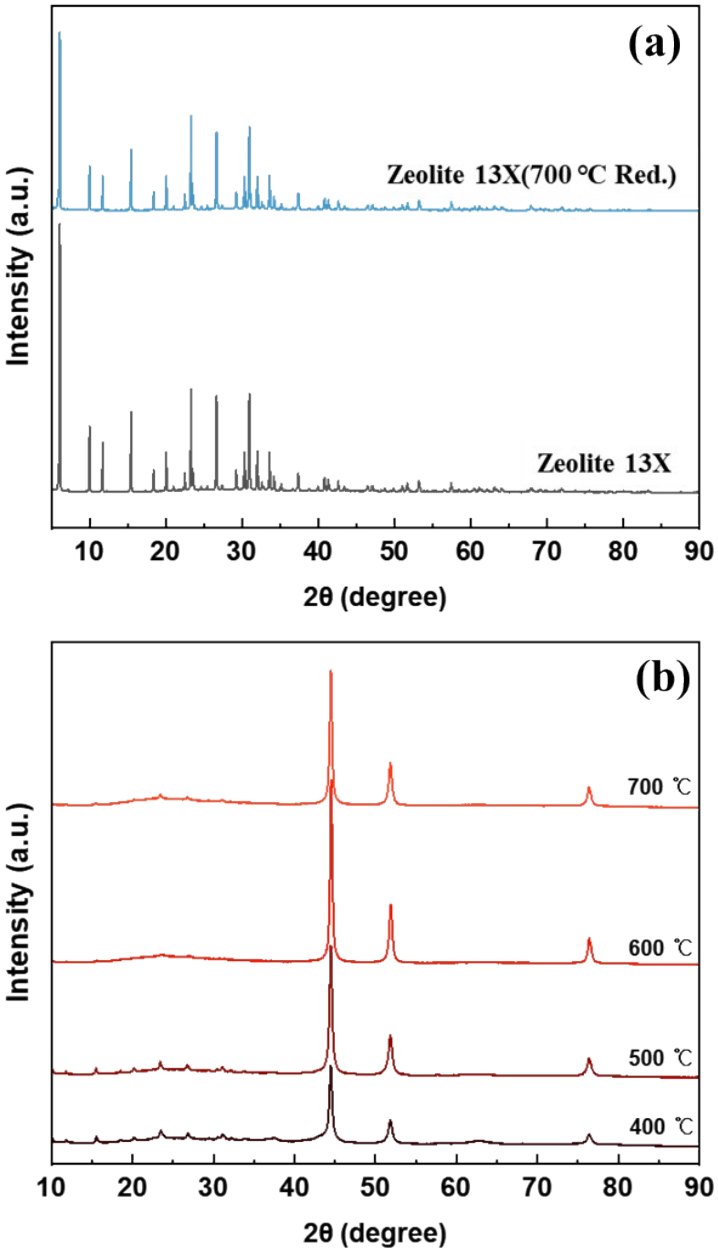

Figure S2. XRD patterns of (a) fresh and reduced (700 °C, 10% H_2/N_2) zeolite 13X and (b) Ni/13X-DP according to reduction temperature (400 – 700 °C).

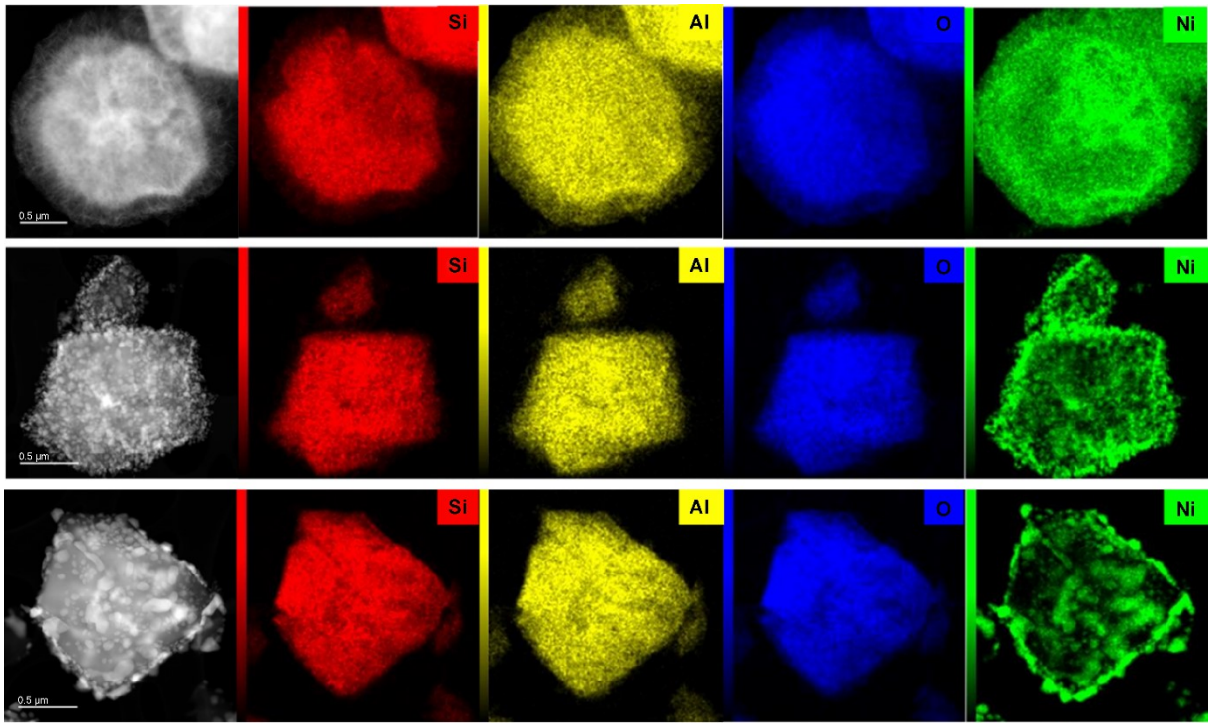

Figure S3. TEM elemental mapping image of recued (a) Ni/13X-IE, (b) Ni/13X-DP, and (c) Ni/13X-IMP.

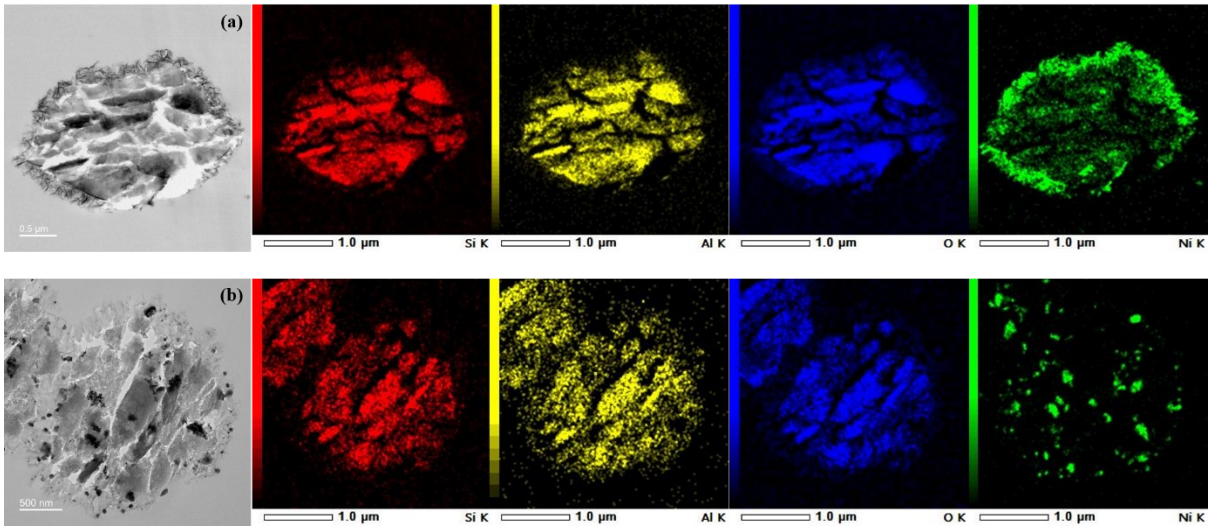

Figure S4. Cross-sectional TEM elemental mapping image of (a) calcined and (b) reduced Ni/13X-DP with ultra-microtome pretreatment.

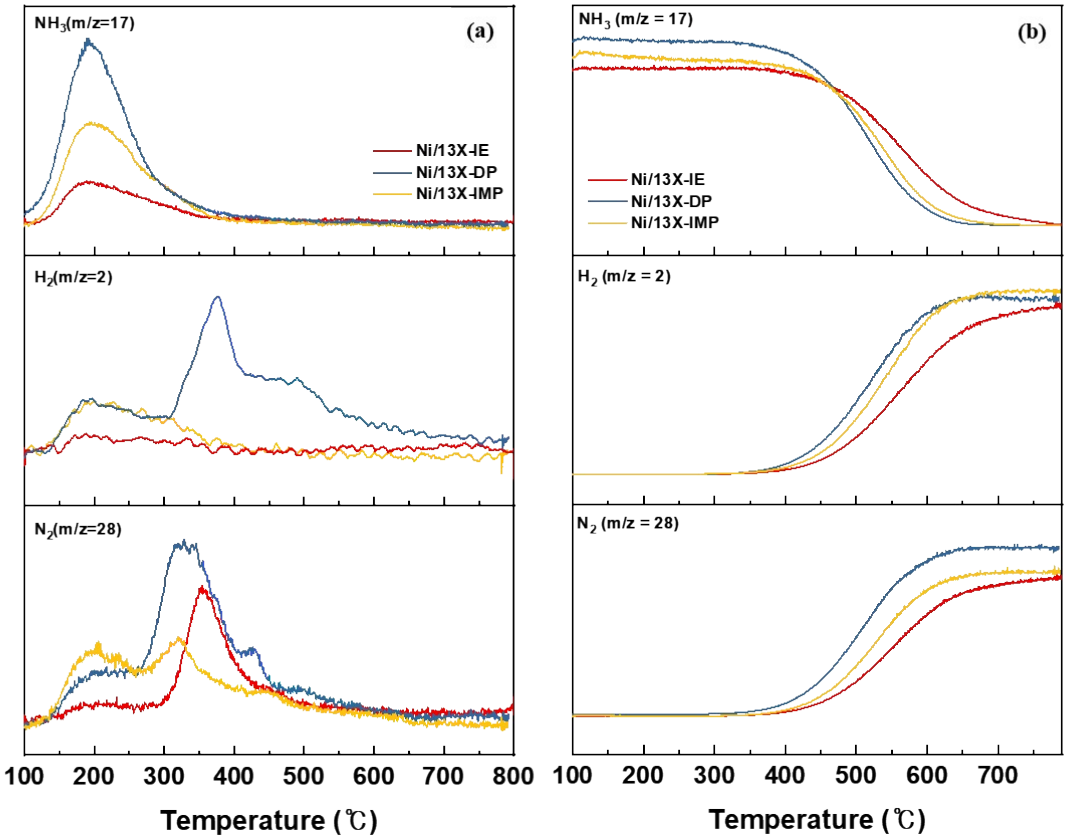

Figure S5. (a) NH_3- TPD-MS and (b) NH_3-TPSR-MS profiles of Ni/zeolite 13X catalysts with different preparation method.

Table S1. H_2 reduction temperature peak of Ni/zeolite 13X catalysts

Ni/zeolite 13X catalyst	Peak α		Peak β		Peak γ	
	Temp. (°C)	Fraction (%)	Temp. (°C)	Fraction (%)	Temp. (°C)	Fraction (%)
Ni/13X-IE	381	0.99	541	36.97	651	62.04
Ni/13X-DP	381	17.84	545	70.72	709	11.44
Ni/13X-IMP	378	71.17	589	28.83	-	-

Table S2. Comparison of catalytic performance of Ni-based catalysts for NH_3 decomposition at 600 °C and WHSV of 30000 mL g_{cat}^{-1} h^{-1}.

Number	Catalyst	Ni loading (wt%)	Method	NH_3 Conversion (%)	H_2 Formation rate (mmol g_{cat}^{-1} min^{-1})	Ref.
1	Ni/MRM-600	15.0	Precipitation	55.0	18.4	1
2	Ni/SiO_2	10.0	Wet impregnation	36.4	11.4	2
3	S60/1.0Mg/10Ni/USY	10	Surfactant-assisted melt infiltration	52	-	3
4	Ni/rGO	25	Sonication	74.2	24.8	4
5	Ni/AC	10	Sonication	40.9	13.7	4
6	Ni/BN	8.9	Sol-gel method	48.1	16.1	5
7	Ni/SiO_2-AEH	10.0	ammonia evaporation-hydrothermal	50	16	6
8	Ni/13X-DP	14.8	Deposition Precipitation	68.3	22.9	This work

References

1. J.-L. Cao, Z.-L. Yan, Q.-F. Deng, Z.-Y. Yuan, Y. Wang, G. Sun, X.-D. Wang, B. Hari and Z.-Y. Zhang, *Catal. Sci. Technol.*, 2014, **4**, 361.

2. T.V Choudhary, C. Sivadinarayana and D. W. Goodman, *Catal. Lett.*, 2001, **72**, 197.

3. E. H. Cho, N. Jeon, B. S. Yoon, S. Kim, Y. Yun and C. H. Ko, *Appl. Surf. Sci.*, 2023, **608**, 155244.

4. T. Meng, Q.-Q. Xu, Y.-T. Li, J.-L. Chang, T.-Z. Ren and Z.-Y. Yuan, *J. Ind. Eng. Chem.*, 2015, **32**, 373.

5. C. Zhou, K. Wu, H. Huang, C.-F. Cao, Y. Luo, C.-Q. Chen, …L. Lin, C. Au and L. Jiang, L. *ACS Catal.*, 2021, **11**, 10345.

6. H. Ren, J. Cheng, H. Fang, F. Zhong, C. Chen, L. Lin and X. Lin, *Appl. Catal. A*, 2023, **664,** 119344.