Supporting Information

FeMo-N nanosheet arrays supported on nickel foam for efficient electrocatalytic reduction of N_2 to NH_3 at ambient condition

Kun Jiang, Kai Li, Shuirong Li, Yan Li, Tao Li, Yun-Quan Liu*, Duo Wang, and Yueyuan Ye

College of Energy, Xiamen University, Xiamen 361102, China.

*Corresponding author.

E-mail address: yq_liu@xmu.edu.cn (Yun-Quan Liu)

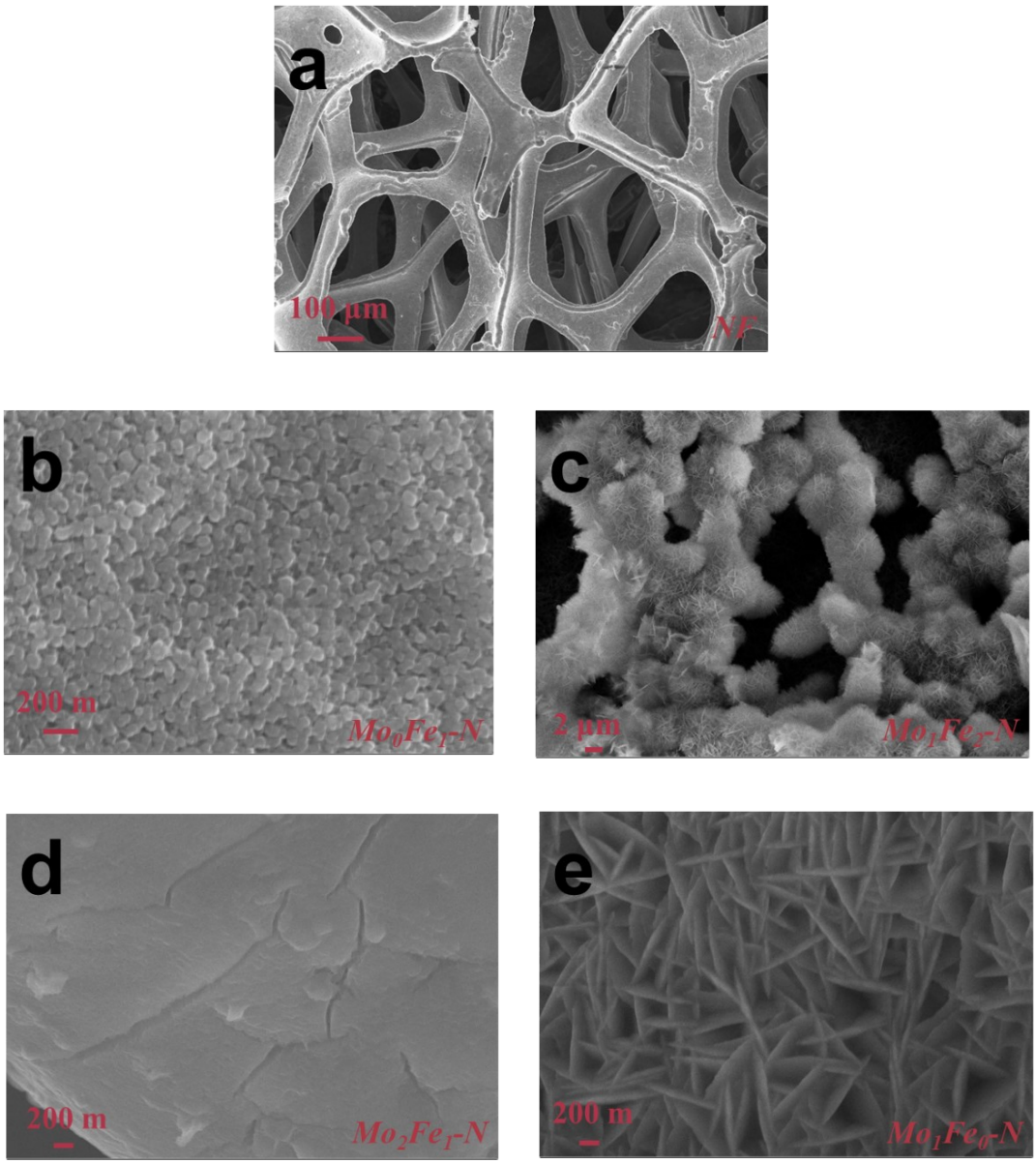


Figure. S1 SEM images for NF and for Fe_mMo_n-N at other molar ratios.

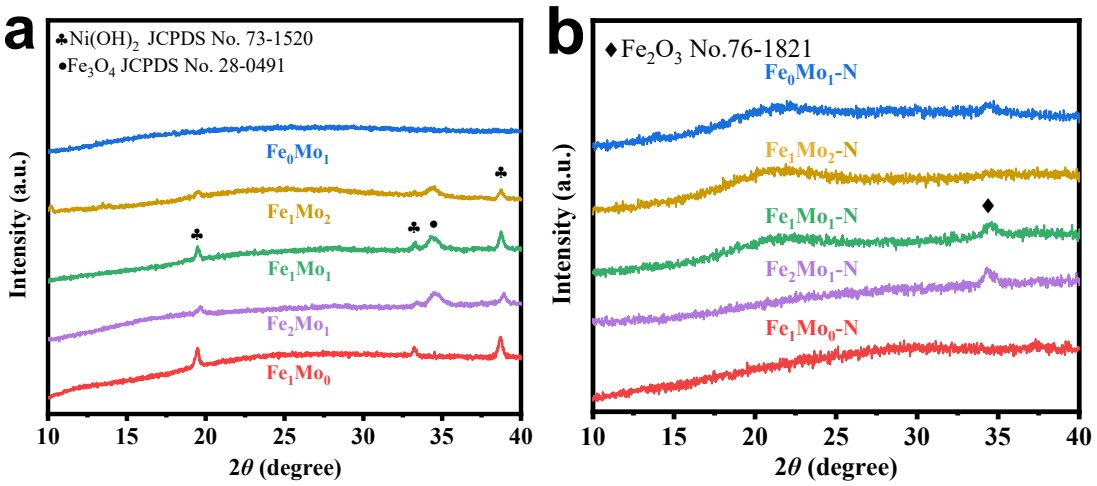


Figure. S2 XRD patterns of (a) Fe_mMo_n and (b) Fe_mMo_n-N.

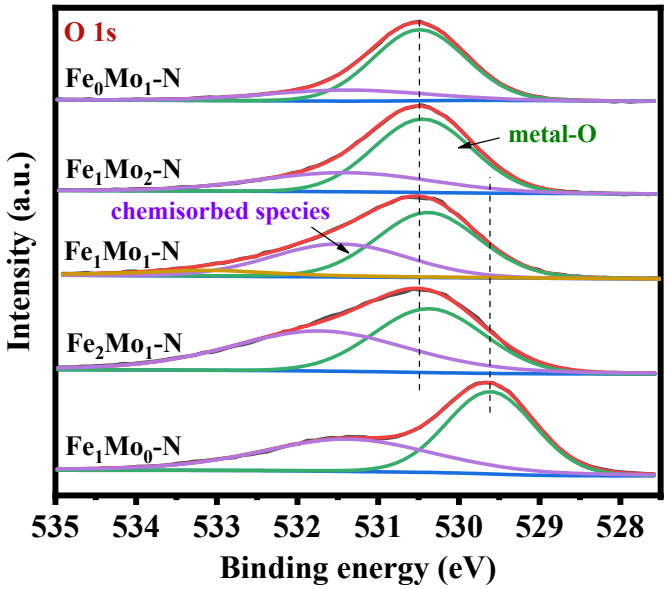


Figure. S3 High-resolution XPS spectra of O 1s for Fe_mMo_n-N.

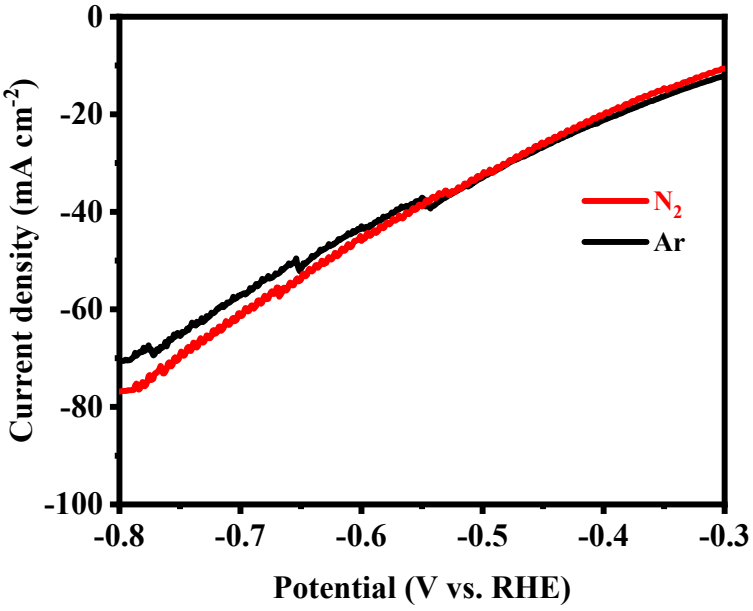


Figure. S4 LSV curves of Fe_1Mo_1-N for NRR in N_2- (red line) and Ar- (black line) saturated electrolytes with a scan rate of 5 mV s^{-1}.

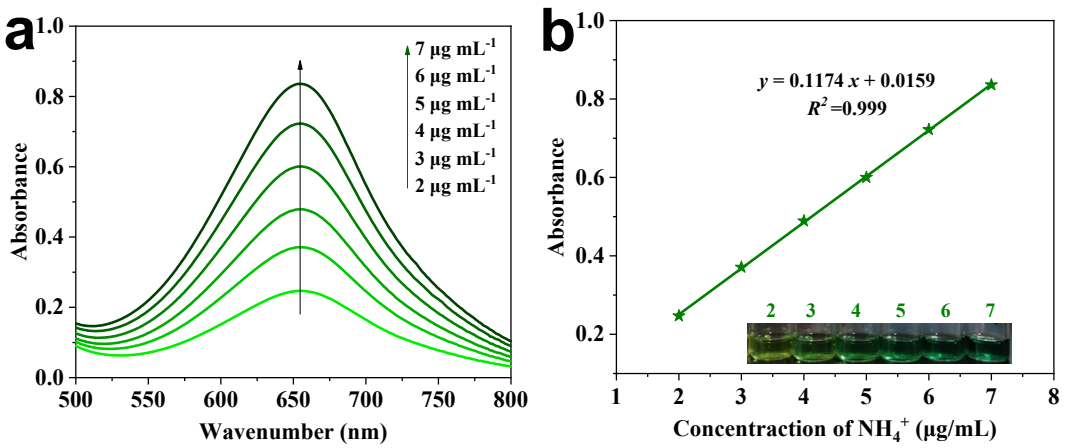


Figure. S5 (a) UV-Vis spectra of indophenol assays with NH_4^+ concentrations after incubated for 2 h at room temperature. (b) Calibration curve used for calculation of NH_4^+ concentrations.

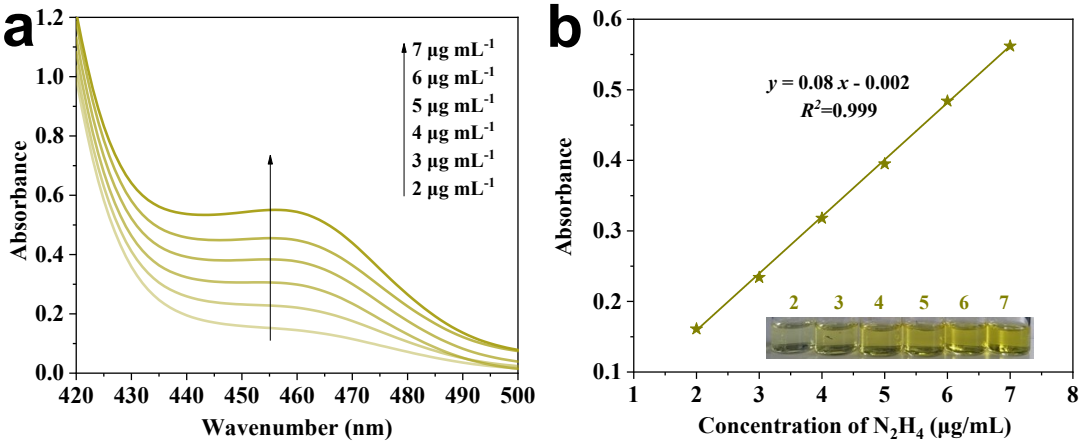


Figure. S6 (a) UV-Vis adsorption spectra of various N_2H_4 concentrations after incubated for 10 min at room temperature. (b) Calibration curve used for calculation of N_2H_4 concentrations.

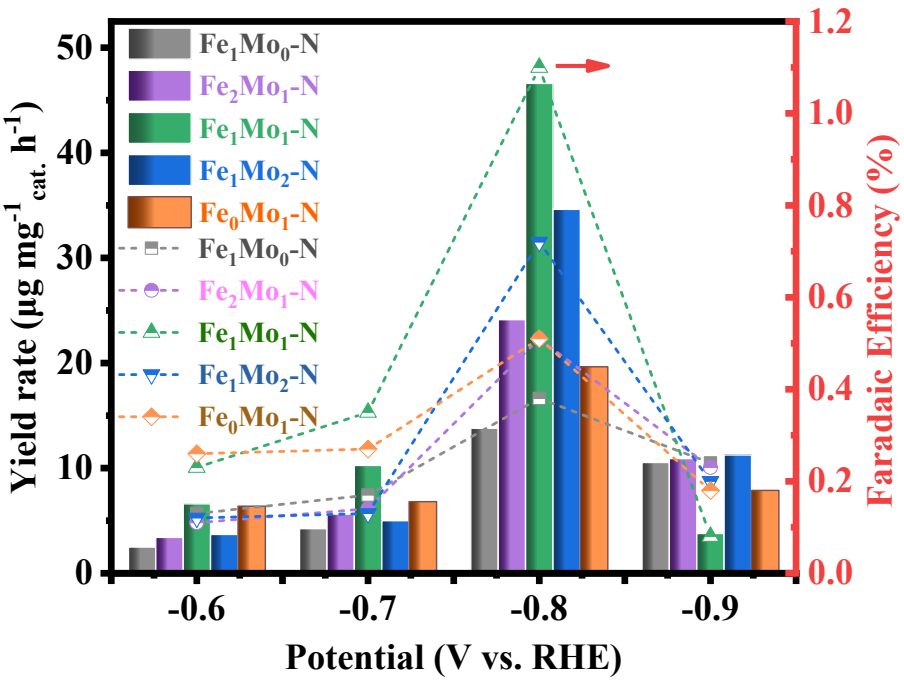
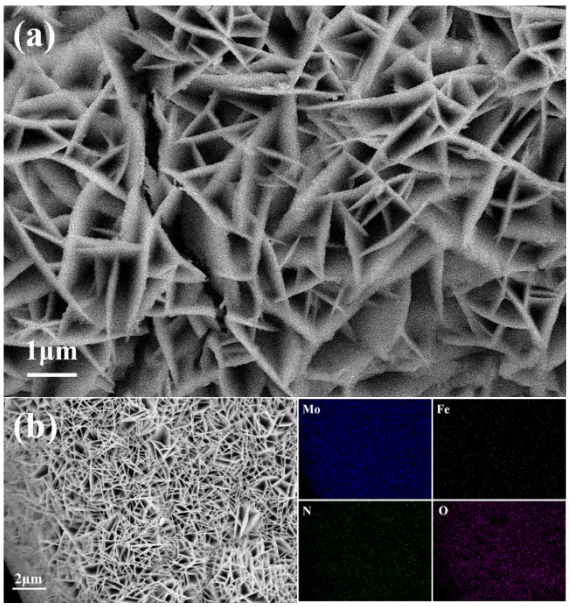
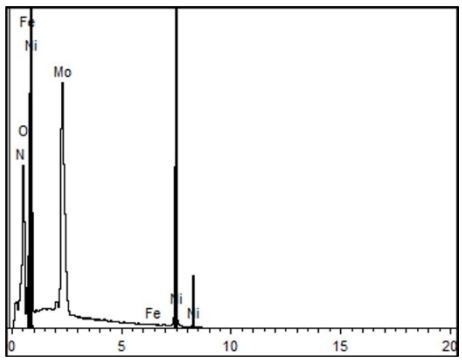


Figure. S7 NH_3 yield rates and FEs of different molar ratios of Fe_mMo_n-N in 0.05 M H_2SO_4 at different potentials.





(d)

Element	Wt. %	At. %
Mo L	37.73	15.28
Fe L	39.34	26.04
N K	8.63	23.95
O K	14.30	34.73

Figure. S8 (a) nanostructure image; (b) element mapping; (c) element spectrum; (d) element content of SEM of Fe_1Mo_1-N after 10 h chronoamperometry test.

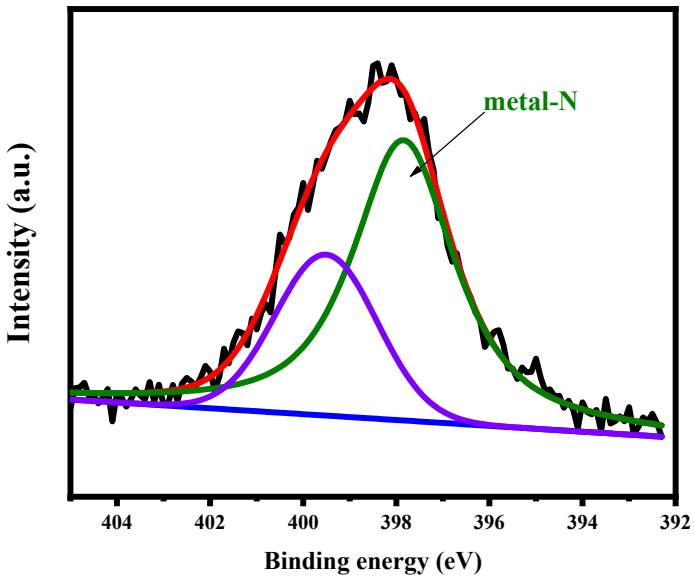


Figure. S9 XPS spectra in N 1s region for Fe_1Mo_1-N after 10 h chronoamperometry in Ar-saturated 0.05 M H_2SO_4 electrolyte.

Table. S1. Elemental atom ratio of Fe_mMo_n-N determined by XPS peak area.

Sample	Mo^{4+}/Mo^{6+}	Fe^{2+}/Fe^{3+}	N atomic %	N atomic of M-N %
Fe_1Mo_0-N	/	0.97	**1.83**	/
Fe_2Mo_1-N	0.99	1.00	**19.51**	10.77
Fe_1Mo_1-N	0.96	1.00	**32.14**	18.52
Fe_1Mo_2-N	1.09	1.00	**29.04**	16.66
Fe_0Mo_1-N	1.22	/	**26.11**	14.67

Table S2. Comparison of the NH_3 yield rate and FE of Fe_1Mo_1-N with other reported NRR electrocatalysts under ambient atmosphere.

Catalyst	Electrolyte	NH_3 yield/μg $mg^{-1}_{mg.}$ h^{-1}	FE/%	Reference
Fe_1Mo_1-N	**0.05 M H_2SO_4**	**46.64**	**1.43**	**This work**
FeTPPCl	0.1 M Na_2SO_4	18.28	16.76	[1][1]
BCN	0.05M Na_2SO_4	41.9	9.87	[2][2]
P-TiO_2	0.1 M $LiClO_4$	23.05	12.26	[3][3]
PdPb/C	0.1 M HCl	37.68	5.79	[4][4]
Ru-NC	0.1 KOH	16.68	14.23	[5][5]
Fe-$(O\text{-}C_2)_4$	0.1 KOH	32.1	29.3	[6][6]
Fe/Mo_2C	0.5 M Na_2SO_4	~37	20.1	[7][7]
Mo-FeS_2	0.1 KOH	26.15	14.41	[8][8]
NiFe-NF	0.1 M Na_2SO_4	16.89	12.50	[9][9]
Mo_2CTX	0.5 M K_2SO_4	40.57	25.77	[10][10]
CN/C	2 M H_2SO_4	2.9	62.1	[11][11]
Mo-Mo_2C/NCNTs	0.005 M H_2SO_4	16.1	7.1	[12][12]
Cu_9S_5	0.5 M Na_2SO_4	10.8	35	[13][13]
$CaCoO_x$	0.05 M Na_2SO_4	16.25	20.51	[14][14]
β-FeOOH	0.5 M $LiClO_4$	42.38	9.02	[15][15]

Notes and References

1. X. X. Yang, S. Sun, L. Meng, K. Li, S. Mukherjee, X. Y. Chen, J. Q. Lv, S. Liang, H. Y. Zang, L. K. Yan and G. Wu, *Applied Catalysis B-Environmental*, 2021, **285**, 119794.
2. B. Chang, L. L. Li, D. Shi, H. H. Jiang, Z. Z. Ai, S. Z. Wang, Y. L. Shao, J. X. Shen, Y. Z. Wu, Y. L. Li and X. P. Hao, *Applied Catalysis B-Environmental*, 2021, **283**, 119622.
3. P. Zhao, L. Zhang, J. Song, S. Wen and Z. Cheng, *Applied Surface Science*, 2020, **523**, 146517.
4. H. Zhao, D. Zhang, Z. C. Wang, Y. Han, X. M. Sun, H. D. Li, X. K. Wu, Y. Pan, Y. N. Qin, S. Y. Lin, Z. K. Xu, J. P. Lai and L. Wang, *Applied Catalysis B-Environmental*, 2020, **265**, 118411.
5. Z. Q. Zhang, K. D. Yao, L. C. Cong, Z. C. Yu, L. N. Qu and W. M. Huang, *Catalysis Science & Technology*, 2020, **10**, 1336-1342.
6. S. B. Zhang, M. Jin, T. F. Shi, M. M. Han, Q. Sun, Y. Lin, Z. H. Ding, L. R. Zheng, G. Z. Wang, Y. X. Zhang, H. M. Zhang and H. J. Zhao, *Angewandte Chemie-International Edition*, 2020, **59**, 13423-13429.
7. T. T. Wang, Z. K. Kou, J. Zhang, H. D. Wang, Y. J. Zeng, S. R. Wei and H. Zhang, *Chemical Engineering Journal*, 2021, **417**, 127924.
8. H. B. Wang, J. Q. Wang, R. Zhang, C. Q. Cheng, K. W. Qu, Y. J. Yang, J. Mao, H. Liu, M. Du, C. K. Dong and X. W. Du, *Acs Catalysis*, 2020, **10**, 4914-4921.
9. Y. Sun, T. Jiang, J. Duan, L. Jiang, X. Hu, H. Zhao, J. Zhu, S. Chen and X. Wang, *ACS Catalysis*, 2020, **10**, 11371-11379.
10. W. Peng, M. Luo, X. D. Xu, K. Jiang, M. Peng, D. C. Chen, T. S. Chan and Y. W. Tan, *Advanced Energy Materials*, 2020, **10**, 2001364.
11. G. M. Peng, J. W. Wu, M. Z. Wang, J. Niklas, H. Zhou and C. Liu, *Nano Lett*, 2020, **20**, 2879-2885.
12. Y. Ma, T. Yang, H. Zou, W. Zang, Z. Kou, L. Mao, Y. Feng, L. Shen, S. J. Pennycook, L. Duan, X. Li and J. Wang, *Adv Mater*, 2020, **32**, 2002177.
13. H. S. Kim, J. Choi, J. Kong, H. Kim, S. J. Yoo and H. S. Park, *Acs Catalysis*, 2021, **11**, 435-445.
14. X. Y. Chen, K. Li, X. X. Yang, J. Q. Lv, S. Sun, S. Q. Li, D. M. Cheng, B. Li, Y. G. Li and H. Y. Zang, *Nano Research*, 2021, **14**, 501-506.
15. X. Zhu, Z. Liu, H. Wang, R. Zhao, H. Chen, T. Wang, F. Wang, Y. Luo, Y. Wu and X. Sun,

Chem Commun (Camb), 2019, **55**, 3987-3990.