

## Supporting information

### Nitrogen Vacancy Rich Molybdenum Nitride Nanosheets as Highly Efficient Electrocatalysts for Nitrogen Reduction Reaction

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**Table S1:** Comparison of the NRR performance of MoN-NV<sub>2</sub> with other recently reported electrocatalysts.

Catalyst	Electrolyte	NH <sub>3</sub> Yield ( $\mu\text{g h}^{-1} \text{mg}^{-1} \text{cat}$ )	FE (%)	Ref.
Mo nanofilm	0.1 M H <sub>2</sub> SO <sub>4</sub>	3.09	0.72	1
MoN nanosheets	0.1 M HCl	3.3	1.15	2
MoN	0.1 M HCl	3.0	1.2	3
VN	0.1 M HCl	8.4	2.3	4
W <sub>2</sub> N <sub>3</sub>	0.1 M KOH	11.7	11.7	5
Mo <sub>2</sub> C/C	0.1 M Li <sub>2</sub> SO <sub>4</sub>	11.3	7.8	6
MoO <sub>3</sub>	0.1 M HCl	29.43	1.9	7
N-doped carbon	0.05 M H <sub>2</sub> SO <sub>4</sub>	11.76	1.42	8
Fe <sub>2</sub> O <sub>3</sub> -CNT	2.0 M NaHCO <sub>3</sub>	0.22	0.15	9
MoS <sub>2</sub>	0.1 Na <sub>2</sub> SO <sub>4</sub>	8.08	1.17	10
MoN-NV <sub>2</sub>	0.1 M KOH	22.5	14	This work

## References

1. Yang, D.; Chen, T.; Wang, Z., Electrochemical reduction of aqueous nitrogen (N2) at a low overpotential on (110)-oriented Mo nanofilm. *J. Mater. Chem. A*. 2017, 5 (36), 18967-18971.
2. Zhang, L.; Ji, X.; Ren, X.; Luo, Y.; Shi, X.; Asiri, A. M.; Zheng, B.; Sun, X., Efficient electrochemical N2 reduction to NH3 on MoN nanosheets array under ambient conditions. *ACS Sustain. Chem. Eng.* 2018, 6 (8), 9550-9554.
3. Li, Q.; He, L.; Sun, C.; Zhang, X., Computational study of MoN2 monolayer as electrochemical catalysts for nitrogen reduction. *J. Phy. Chem. C*. 2017, 121 (49), 27563-27568.

4. Zhang, R.; Zhang, Y.; Ren, X.; Cui, G.; Asiri, A. M.; Zheng, B.; Sun, X., High-efficiency electrosynthesis of ammonia with high selectivity under ambient conditions enabled by VN nanosheet array. *ACS Sustain. Chem. Eng.* 2018, 6 (8), 9545-9549
5. Jin, H.; Li, L.; Liu, X.; Tang, C.; Xu, W.; Chen, S.; Song, L.; Zheng, Y.; Qiao, S.-Z., Nitrogen vacancies on 2D layered W<sub>2</sub>N<sub>3</sub>: A Stable and efficient active site for nitrogen reduction reaction. *Adv. Mater.* 2019, 31 (32), 1902709.
6. Cheng, H.; Ding, L. X.; Chen, G. F.; Zhang, L.; Xue, J.; Wang, H., Molybdenum carbide nanodots enable efficient electrocatalytic nitrogen fixation under ambient conditions. *Adv. Mater.* 2018, 30 (46), 1803694.
7. Han, J.; Ji, X.; Ren, X.; Cui, G.; Li, L.; Xie, F.; Wang, H.; Li, B.; Sun, X., MoO<sub>3</sub> nanosheets for efficient electrocatalytic N<sub>2</sub> fixation to NH<sub>3</sub>. *J. Mater. Chem. A.* 2018, 6 (27), 12974-12977.
8. Liu Y, Su Y, Quan X, Fan X, Chen S, Yu H, Zhao H, Zhang Y, Zhao J. Facile ammonia synthesis from electrocatalytic N<sub>2</sub> reduction under ambient conditions on N-doped porous carbon. *ACS Catal.* 2018, 8(2), 1186-91.
9. Chen S, Perathoner S, Ampelli C, Mebrahtu C, Su D, Centi G. Electrocatalytic synthesis of ammonia at room temperature and atmospheric pressure from water and nitrogen on a carbon-nanotube-based electrocatalyst. *Angewandte Chemie International Edition*. 2017, 56(10), 2699-703.
10. Zhang, L., Ji, X., Ren, X., Ma, Y., Shi, X., Tian, Z., Asiri, A.M., Chen, L., Tang, B. and Sun, X. Electrochemical ammonia synthesis via nitrogen reduction reaction on a MoS<sub>2</sub> catalyst: theoretical and experimental studies. *Advanced Materials*, 2018, 30 (28), 1800191.