Table S2. Comparison of the NO_3RR activity and NH_3 yield performance among nitrogen-doped carbon-supported Co NPs and the recently reported M-N-C-based electrocatalyst.

Catalysts	Electrolyte	Potential (V vs. RHE)	FE_{NH3} (%)	NH_3 yield	Ref.
Co NPs	1 M KOH + 0.5 M KNO_3	-0.4 V	98.07	31.891 mg h^{-1} mg_{cat}^{-1}	This work
Non-noble metal-based single-atom catalysts					
Cu-CN_4	0.1 M KOH + 0.1 M KNO_3	-1.0 V	84.7	4.5 mg $cm^{-2}h^{-1}$	[7]
Cu-CN_3	0.05 M Na_2SO_4 + 1.6 mM $NaNO_3$	-0.64 V	65.3	50.3 μmol $g_{cat}^{-1}h^{-1}$	[8]
Cu-CN_3 SACs/NCNT	1 M KOH + 1 M KNO_3	-0.8 V	89.64	30.09 mg $mg_{cat}^{-1}h^{-1}$	[9]
Fe SAC	0.1 M K_2SO_4+ 0.5 M KNO_3	-0.66 V	75	20 mg $cm^{-2}h^{-1}$	[10]
FeN_2O_2 SAC	0.1 M Na_2SO_4 + 0.5 M KNO_3	-0.68 V	92	9.2 mg $cm^{-2}h^{-1}$	[11]
$FeCN_3$ SAC	0.1 M K_2SO_4 + 0.5 M KNO_3	-0.7 V	86	18 mg $mg_{cat}^{-1}h^{-1}$	[12]
2D Fe- SACs	0.1 M KOH + 0.1 M KNO_3	-0.4 V	95.4	68.6 mg $mg_{cat}^{-1}h^{-1}$	[13]
Co-CNP	0.02 M Na_2SO_4 + 100 mg/L $NaNO_3$	-0.69 V	92.0	0.43 mg $cm^{-2}h^{-1}$	[14]
ZnNC-900	1 M KOH + 0.1 M KNO_3	-0.7 V	~90	1.29 mmol $cm^{-2}h^{-1}$	[15]
ZnSA-MNC	0.1 M Na_2SO_4 + 0.5 M $NaNO_3$	-0.9 V	94.8	39 mg $mg_{cat}^{-1}h^{-1}$	[16]
NiNPs@NiSAs-NCNTs/CC	0.5 M Na_2SO_4 + 0.3 M $NaNO_3$	-1.4 V	100	27.67 mg $cm^{-2}h^{-1}$	[17]
Noble metal-based single-atom catalysts					
Ag_1/NOCNT	0.5 M Na_2SO_4 + 50 mM $NaNO_3$	-0.5 V	93.4	1.33 mol $g_{cat}^{-1}h^{-1}$	[18]
Ru_1-TiO_x/Ti	1 M KOH + 0.5 M $NaNO_3$	-0.3 V	87.6	22.2 mol $g^{-1}h^{-1}$	[19]
Ru SAs-Co_3O_4	1 M KOH + 0.1 M KNO_3	-0.5 V	94.92	1.843 mmol $cm^{-2}h^{-1}$	[20]
Ru SA-NC	1 M KOH + 0.5 M KNO_3	-0.6 V	72.8	0.134 mmol $cm^{-2}h^{-1}$	[21]
Bi-N-C	0.5 M KOH + 0.5 M KNO_3	-0.35 V	88.7	1.38 mg $mg_{cat}^{-1}h^{-1}$	[22]
Rh@Cu-0.6%	0.1 M Na_2SO_4 + 0.1 M KNO_3	-0.2 V	93	1.27 mmol $cm^{-2}h^{-1}$	[23]
Au/Cu SAA	0.5 M Na_2SO_4 + 100 ppm $NaNO_3$	-0.8 V	99.69	0.193 mmol $cm^{-2}h^{-1}$	[24]
Cluster-based catalysts					
Pd_{10}Cu/BCN	1 M KOH + 100 mM KNO_3	-0.6 V	91.47	102.15 mg $mg_{cat}^{-1}h^{-1}$	[25]
CuPd/CN	0.5 M K_2SO_4 + 200 ppm KNO_3	-0.46 V	96.16	1.5368 mg $mg_{cat}^{-1}h^{-1}$	[26]
Ru NCs/TO_2 NTs	0.05 M Na_2SO_4 + 100 ppm $NaNO_3$	-0.4 V	90	0.600 mg $cm^{-2}h^{-1}$	[27]
Au-NC/TiO_2	0.2 M Na_2SO_4 + 0.05 M $NaNO_3$	-0.6 V	91	1.923 mg $mg_{cat}^{-1}h^{-1}$	[28]
BCN@Ni	0.1 M KOH + 100 mM KNO_3	-0.3 V	91.15	2.32 mg $cm^{-2}h^{-1}$	[29]
B@GO	0.1 M K_2SO_4 + 0.5 M KNO_3	-0.8 V	61.88	40 mg $mg_{cat}^{-1}h^{-1}$	[30]
CuCN/NHCSs	0.1 M KOH + 0.1 M KNO_3	-1.1 V	91.08	21.4 mg $mg_{cat}^{-1}h^{-1}$	[31]

References

1. Furthmuller GKJ. 1996. Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set. *PHYSICAL REVIEW B* 54:11169-86

2. Ernzerhof JPPKBM. 1996. Generalized Gradient Approximation Made Simple. *Physical Review Letters* 77:3868

3. Grimme S. 2006. Semiempirical GGA-type density functional constructed with a long-range dispersion correction. *J Comput Chem* 27:1787-99

4. Tang W, Sanville E, Henkelman G. 2009. A grid-based Bader analysis algorithm without lattice bias. *J Phys Condens Matter* 21:084204

5. Guo S, Heck K, Kasiraju S, Qian H, Zhao Z, et al. 2017. Insights into Nitrate Reduction over Indium-Decorated Palladium Nanoparticle Catalysts. *ACS Catalysis* 8:503-15

6. Liu J-X, Richards D, Singh N, Goldsmith BR. 2019. Activity and Selectivity Trends in Electrocatalytic Nitrate Reduction on Transition Metals. *ACS Catalysis* 9:7052-64

7. Yang J, Qi H, Li A, Liu X, Yang X, et al. 2022. Potential-Driven Restructuring of Cu Single Atoms to Nanoparticles for Boosting the Electrochemical Reduction of Nitrate to Ammonia. *J Am Chem Soc* 144:12062-71

8. Xue Y, Yu Q, Ma Q, Chen Y, Zhang C, et al. 2022. Electrocatalytic Hydrogenation Boosts Reduction of Nitrate to Ammonia over Single-Atom Cu with Cu(I)-N(3)C(1) Sites. *Environ Sci Technol* 56:14797-807

9. Wang Y, Zhang WC, Wen WD, Yu XY, Du YX, et al. 2023. Atomically Dispersed Unsaturated Cu-N Sites on High-Curvature Hierarchically Porous Carbon Nanotube for Synergetic Enhanced Nitrate Electroreduction to Ammonia. *Advanced Functional Materials* 33

10. Moore GWK, Howell SEL, Brady M, Xu X, McNeil K. 2021. Anomalous collapses of Nares Strait ice arches leads to enhanced export of Arctic sea ice. *Nat Commun* 12:1

11. Zhang WD, Dong HL, Zhou L, Xu HW, Wang HR, et al. 2022. Fe single-atom catalysts with pre-organized coordination structure for efficient electrochemical nitrate reduction to ammonia. *Applied Catalysis B-Environment and Energy* 317

12. Liu L, Xiao T, Fu H, Chen Z, Qu X, Zheng S. 2023. Construction and identification of highly active single-atom Fe1-NC catalytic site for electrocatalytic nitrate reduction. *Applied Catalysis B: Environmental* 323

13. Li J, Zhong WQ, Wu K, Petit E, Lajaunie L, et al. 2024. Efficient solar-driven electrocatalytic nitrate-to-ammonia conversion by 2D ultrathin Fe single-atom catalysts. *Journal of Materials Chemistry A* 12:26103-12

14. Li J, Li M, An N, Zhang S, Song Q, et al. 2022. Boosted ammonium production by single cobalt atom catalysts with high Faradic efficiencies. *Proc Natl Acad Sci U S A* 119:e2123450119

15. Li Q, Ma Y, Zeng Q, Liu W, Wang C, et al. 2025. Coupling ZnN(4) Atomic Sites with Graphitic Nitrogen for Enhanced Ammonium Production via Electrocatalytic Nitrate Reduction. *Small* 21:e2409925

16. Zhao J, Ren X, Liu X, Kuang X, Wang H, et al. 2023. Zn single atom on N-doped carbon: Highly active and selective catalyst for electrochemical reduction of nitrate to ammonia. *Chemical Engineering Journal* 452

17. Xi ZC, Wang JQ, Liu BC, Xu X, Jing P, et al. 2023. Elaborately tuning the electronic structure of single-atom nickel sites using nickel nanoparticles to markedly enhance the electrochemical reduction of nitrate into ammonia. *Journal of Energy Chemistry* 83:32-42

18. Shen Z, Yu YS, Zhao ZW, Mushtaq MA, Ji QQ, et al. 2023. N, O trans-coordinating silver single-atom catalyst for robust and efficient ammonia electrosynthesis from nitrate. *Applied Catalysis B-Environment and Energy* 331

19. Yao Y, Zhao L, Dai J, Wang J, Fang C, et al. 2022. Single Atom Ru Monolithic Electrode for Efficient Chlorine Evolution and Nitrate Reduction. *Angew Chem Int Ed Engl* 61:e202208215

20. Xu SX, Zhu Y, Wen ZB, Yu SM, Teng ZY, et al. 2023. Modulating the proton transfer kinetics via Ru

single atoms for highly efficient ammonia synthesis. *Chem Catalysis* 3

21. Ke Z, He D, Yan X, Hu W, Williams N, et al. 2023. Selective NO(x)(-) Electroreduction to Ammonia on Isolated Ru Sites. *ACS Nano* 17:3483-91

22. Zhang W, Zhan S, Xiao J, Petit T, Schlesiger C, et al. 2023. Coordinative Stabilization of Single Bismuth Sites in a Carbon-Nitrogen Matrix to Generate Atom-Efficient Catalysts for Electrochemical Nitrate Reduction to Ammonia. *Adv Sci (Weinh)* 10:e2302623

23. Liu H, Lang X, Zhu C, Timoshenko J, Ruscher M, et al. 2022. Efficient Electrochemical Nitrate Reduction to Ammonia with Copper-Supported Rhodium Cluster and Single-Atom Catalysts. *Angew Chem Int Ed Engl* 61:e202202556

24. Yin H, Peng Y, Li J. 2023. Electrocatalytic Reduction of Nitrate to Ammonia via a Au/Cu Single Atom Alloy Catalyst. *Environ Sci Technol* 57:3134-44

25. Yang L, Feng S, Zhu W. 2023. Achieving reaction pathway separation for electrochemical nitrate fixation on triatomic catalysts: A new mechanism. *Journal of Hazardous Materials* 441

26. Xu Y, Shi K, Ren T, Yu H, Deng K, et al. 2022. Electronic Metal-Support Interaction Triggering Interfacial Charge Polarization over CuPd/N-Doped-C Nanohybrids Drives Selectively Electrocatalytic Conversion of Nitrate to Ammonia. *Small* 18:e2203335

27. Qiu W, Xie M, Wang P, Gao T, Li R, et al. 2023. Size-Defined Ru Nanoclusters Supported by TiO(2) Nanotubes Enable Low-Concentration Nitrate Electroreduction to Ammonia with Suppressed Hydrogen Evolution. *Small* 19:e2300437

28. Yang MS, Wei TR, He J, Liu Q, Feng LG, et al. 2024. Au nanoclusters anchored on TiO

nanosheets for high-efficiency electroreduction of nitrate to ammonia. *Nano Research* 17:1209-16

29. Zhao X, Zhu Z, He YN, Zhang HB, Zhou XH, et al. 2022. Simultaneous anchoring of Ni nanoparticles and single-atom Ni on BCN matrix promotes efficient conversion of nitrate in water into high-value-added ammonia. *Chemical Engineering Journal* 433

30. Ingavale S, Marbaniang P, Palabathuni M, Kale VN, Mishra N. 2023. Decoration of boron nanoparticles on a graphene sheet for ammonia production from nitrate. *Nanoscale* 15:11497-505

31. Shu Z, Chen HF, Liu X, Jia HX, Yan HJ, Cai YQ. 2023. High-Throughput Screening of Heterogeneous Transition Metal Dual-Atom Catalysts by Synergistic Effect for Nitrate Reduction to Ammonia. *Advanced Functional Materials* 33