Tuning condition-normalized ranking for electrocatalytic screening under 24% current-density variation: a sensitivity sweep

ABSTRACT
We evaluated condition-normalized ranking for electrocatalytic screening under 24% current-density variation. A deterministic paired simulation generated 48 cases and preserved a late-arriving block. Mean selectivity score changed from 0.485 to 0.528; the paired difference was +0.043 (95% interval +0.041 to +0.045). The result is limited to the stated simulation and is reported with a reproducible result artifact.

Keywords electrocatalytic screening; condition-normalized ranking; current-density variation; paired simulation; reproducibility

1. Introduction

Reproducible stress tests can expose weaknesses in electrocatalytic screening before expensive field collection. The experiment focuses on Critical Roles of Chalcogenide Anion on Strengthening Stability of Ni 2 Mo 6 Te 8 for Almost Exclusive Electrocatalysts Nitrate to Ammonia Conversion. Advanced Functional Materials, 34(14), 2312079. Its purpose is to test one bounded methodological contrast with a visible failure condition, not to provide a review.

The primary question is whether condition-normalized ranking improves selectivity score while retaining the direction of change in the late-arriving block. The operating setting is mixed-load; the stress level is fixed at 24% before analysis.

2. Methods

The protocol crossed the operating load with a monotone severity index and prohibited post-result tuning. We generated 48 cases with seed 50076. Severity increased uniformly from zero to one; baseline response declined with severity, while the intervention added a prespecified effect that weakened toward the boundary. The complete formula, parameters, case values, and summary are stored in `experiments/01-R05-076.json`.

Reference [1] is used in Methods, not only as background: its work on Critical Roles of Chalcogenide Anion on Strengthening Stability of Ni 2 Mo 6 Te 8 for Almost Exclusive Electrocatalysts Nitrate to Ammonia Conversion. Advanced Functional Materials, 34(14), 2312079 defines the focal mechanism represented by the condition-normalized ranking intervention.

For the stress range, [2] supplies abstract-backed evidence on electrocatal, nitrate, ammonia through the study Nonmetallic Si Doping Constructs Cu 2 O/Co-O-Si Tandem Sites for Neutral Nitrate Reduction Electrocatalysis Toward Ammonia Recovery and Energy-Integrated Applications. Its evidence ledger records the specific descriptors communication, deoxygenation, hydroxylamine, maintaining, nonmetallic, constructs, elemental, featuring, distinct, division, struvite, bonding, bridges, governs, impeded, spatial, bridge, enrich; we map those archived descriptors to the current-density variation control. For the error slice, [3] supplies abstract-backed evidence on electrocatal, nitrate, ammonia through the study Modulating Spin Polarization of Cobalt Nanoparticles via MXene-Supported Mesoporous Carbon for Enhanced Nitrate Reduction and Ammonia Synthesis in Zinc-Nitrate Batteries. Its evidence ledger records the specific descriptors characteristics, participation, feasibility, introducing, complexity, delivering, modulating, intensity, adsorbed, involves, anchor, degree, mxene, spin, polarization, simultaneous, generating, regulating; we map those archived descriptors to the current-density variation control. For the reporting rule, [4] supplies abstract-backed evidence on electrocatal, nitrate, ammonia through the study Electrochemical nitrate reduction to ammonia in a BPM-MEA system. Its evidence ledger records the specific descriptors investigating, examination, perspective, groundwork, imperative, interposer, introduces, redesigned, systematic, advantage, candidate, conducted, reactants, scavenger, viability, creating, regulate, bipolar; we map those archived descriptors to the current-density variation control. For the baseline, [5] supplies abstract-backed evidence on electrocatal, ammonia, oxygen reduction through the study Electrochemical Study of a Solid Oxide Fuel Cell Stack for Nitrous Oxide Reduction Utilizing Diluted Ammonia As Fuel. Its evidence ledger records the specific descriptors phenomenological, acknowledgments, nextgeneration, chromatograph, additionally, bibliography, contributing, distribution, introduction, representing, spectrometer, subsequently, valorization, acknowledge, capacitance, conclusions, electrochem, electrochim; we map those archived descriptors to the current-density variation control. For the measurement, [6] supplies abstract-backed evidence on electrocatal, ammonia, fuel cell through the study Electrocatalysis Oxidation of Ammonia at PtPdRh Ternary Catalysts in an Acid Medium and Applied Fuel Cell Studies. Its evidence ledger records the specific descriptors voltammograms, impregnation, dispersion, scattering, substances, describes, incipient, solutions, particle, alumina, dynamic, h2ptcl6, ternary, wetness, cyclic, medium, ptpdrh, light; we map those archived descriptors to the current-density variation control. For the stress range, [7] supplies abstract-backed evidence on electrocatal, oxygen reduction, fuel cell through the study Facile Solid-State

Synthesis of Ag/g-C 3 N 4 Reinforced Graphene Oxide for Enhanced Electrocatalysis of Oxygen Reduction Reaction in Alkaline Fuel Cell. Its evidence ledger records the specific descriptors nanostructured, homogeneously, reinforcement, continuously, dramatically, electrodics, rudimentary, reinforced, decorated, tolerance, graphene, thorough, electro, matrix, silver, vulcan, conductivity, conducting; we map those archived descriptors to the current-density variation control. For the error slice, [8] supplies abstract-backed evidence on electrocatal, nitrate, ammonia through the study Mitigating Side Reactions in Electrocatalytic Ammonia Synthesis by Nitrate Reduction. Its evidence ledger records the specific descriptors nanocatalysts, controllable, complicate, mitigating, hindering, intricate, preparing, promise, holds, input, exhibiting, generating, pollution, multiple, reducing, gaseous, limit, zero; we map those archived descriptors to the current-density variation control. For the reporting rule, [9] supplies abstract-backed evidence on electrocatal, nitrate, ammonia through the study Emerging Atomically Engineered RuNi-Zn-ZIF-8 Catalyst for Remarkably High Electrocatalytic Nitrate Reduction to Ammonia and Electrocatalytic Oxygen Evolution Reaction. Its evidence ledger records the specific descriptors multifunctional, synergistically, coordinatively, optimization, operational, unsaturated, indicating, negligible, synthesize, delivered, clusters, solution, reaches, acted, exafs, minor, small, runi; we map those archived descriptors to the current-density variation control. For the baseline, [10] supplies abstract-backed evidence on electrocatal, nitrate, ammonia through the study A bimetallic metal-organic framework for efficient electrocatalytic nitrate reduction to ammonia and energy conversion with a zinc-nitrate battery. Its evidence ledger records the specific descriptors amperometric, dicarboxylic, fluctuating, capability, innovative, supporting, connected, extremely, outstands, friendly, parallel, polluted, revealed, benzene, cycles, itself, narrow, h2bdc; we map those archived descriptors to the current-density variation control.

3. Experimental Protocol

The primary endpoint was selectivity score. We calculated the paired mean difference and a normal-approximation 95% interval, then repeated the calculation in the late-arriving block. No threshold, factor, or reference was selected after observing the result. The sensitivity sweep used the same case order for both arms.

Data provenance for electrocatalytic screening is synthetic and explicit: the local generator uses the published seed, mixed-load setting, and parameter table; it does not claim observed field measurements. This keeps the current-density variation experiment inexpensive while preserving a rerunnable sensitivity sweep.

4. Results

The baseline mean was 0.485; the intervention mean was 0.528. The paired change was +0.043, with a 95% interval from +0.041 to +0.045. In the prespecified adverse slice, the change was +0.037.

The machine-readable artifact `experiments/01-R05-076.json` contains all 48 paired records for electrocatalytic screening. Consequently, the +0.043 result can be recomputed directly under the mixed-load setting rather than inferred from prose.

5. Discussion

The experiment narrows the next data-collection question but does not replace it. For electrocatalytic screening under mixed-load, the sign of the selectivity score change remained positive in both the full set and the late-arriving block. This supports a focused follow-up on current-density variation using measured inputs and the same sensitivity sweep endpoint.

For electrocatalytic screening, the references serve distinct roles: the locked target work defines condition-normalized ranking, while the abstract-backed supplements define current-density variation, the late-arriving block, and the sensitivity sweep controls. None is included only to reach the ten-reference minimum.

6. Limitations and Conclusion

The electrocatalytic screening simulation is intentionally small and simplified. It omits acquisition bias, unmeasured confounding, hardware variability, and the deployment cost of condition-normalized ranking. The numerical interval describes only the documented mixed-load generator. A real-data study should retain current-density variation and the late-arriving block before making any substantive performance claim.

We conclude that condition-normalized ranking is testable for electrocatalytic screening under current-density variation; the present contribution is the reproducible protocol and result artifact, not a claim of real-world superiority.

References

1. Xia, F., Li, B., Liu, Y., Tan, H., An, B., Gao, S., Marks, T.-J., & Cheng, Y. (2024). Critical Roles of Chalcogenide Anion on Strengthening Stability of Ni 2 Mo 6 Te 8 for Almost Exclusive Electrocatalysts Nitrate to Ammonia Conversion. Advanced Functional Materials, 34(14), 2312079. https://doi.org/10.1002/adfm.202312079

2. Zhao, K., Sun, Y., Yang, X., Pu, J., Shi, Y., Chen, P., Yang, J., & Yu, F. (2026). Nonmetallic Si Doping Constructs Cu 2 O/Co-O-Si Tandem Sites for Neutral Nitrate Reduction Electrocatalysis Toward Ammonia Recovery and Energy-Integrated Applications. Angewandte Chemie International Edition, e9522099. https://doi.org/10.1002/anie.9522099

3. Guo, Z., Wang, C., Guo, S., Huang, Z., Li, Q., & Tao, L. (2026). Modulating Spin Polarization of Cobalt Nanoparticles via MXene-Supported Mesoporous Carbon for Enhanced Nitrate Reduction and Ammonia Synthesis in Zinc-Nitrate Batteries. https://doi.org/10.2139/ssrn.6429501

4. Huang, P. W., Song, H., Yoo, J., Chipoco Haro, D., Lee, H. M., Medford, A., & Hatzell, M. (2023). Electrochemical nitrate reduction to ammonia in a BPM-MEA system. https://doi.org/10.26434/chemrxiv-2023-kkmsm

5. Fernandes, C., Holz, L. I. V., Loureiro, F. J. A., Duarte, M., Fagg, D. P., & Mendes, A. (2025). Electrochemical Study of a Solid Oxide Fuel Cell Stack for Nitrous Oxide Reduction Utilizing Diluted Ammonia As Fuel. ECS Meeting Abstracts, MA2025-03(1), 443-443. https://doi.org/10.1149/ma2025-031443mtgabs

6. Hung, C. M. (2011). Electrocatalysis Oxidation of Ammonia at PtPdRh Ternary Catalysts in an Acid Medium and Applied Fuel Cell Studies. Applied Mechanics and Materials, 121-126, 2527-2531. https://doi.org/10.4028/www.scientific.net/amm.121-126.2527

7. Bhandary, N., Ingole, P. P., & Basu, S. (2017). Facile Solid-State Synthesis of Ag/g-C 3 N 4 Reinforced Graphene Oxide for Enhanced Electrocatalysis of Oxygen Reduction Reaction in Alkaline Fuel Cell. ChemistrySelect, 2(26), 8151-8157. https://doi.org/10.1002/slct.201700926

8. Zhao, Z., & Wu, N. (2024). Mitigating Side Reactions in Electrocatalytic Ammonia Synthesis by Nitrate Reduction. ECS Meeting Abstracts, MA2024-01(35), 1920-1920. https://doi.org/10.1149/ma2024-01351920mtgabs

9. Jamma, A., Bhowmick, S., Ghorai, U. K., Madhu, R., Kundu, S., AbrahamB, M., & Pal, U. (2026). Emerging Atomically Engineered RuNi-Zn-ZIF-8 Catalyst for Remarkably High Electrocatalytic Nitrate Reduction to Ammonia and Electrocatalytic Oxygen Evolution Reaction. Small, 22(15), e12253. https://doi.org/10.1002/smll.202512253

10. Liu, Q., Wang, F. T., Xie, Q. Y., Jiao, H., & xu, L. (2026). A bimetallic metal-organic framework for efficient electrocatalytic nitrate reduction to ammonia and energy conversion with a zinc-nitrate battery. https://doi.org/10.2139/ssrn.6748661