Measuring condition-normalized ranking for electrocatalytic screening under 30% current-density variation: a sensitivity sweep

ABSTRACT
We evaluated condition-normalized ranking for electrocatalytic screening under 30% current-density variation. A deterministic paired simulation generated 64 cases and preserved a upper-severity quartile. Mean selectivity score changed from 0.520 to 0.561; the paired difference was +0.041 (95% interval +0.039 to +0.044). 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

Method comparisons in electrocatalytic screening need an adverse slice as well as an overall average. 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 upper-severity quartile. The operating setting is burst-load; the stress level is fixed at 30% before analysis.

2. Methods

A small simulated benchmark separated the intervention effect from case-order and sampling effects. We generated 64 cases with seed 50126. 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-R05-126.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 Ultralow overpotential nitrate reduction to ammonia via a three step relay mechanism. Its evidence ledger records the specific descriptors agriculture, extended, adopted, records, issue, sold, overpotential, simulations, spontaneous, composed, designed, overcome, ultralow, alloys, versus, leads, onset, plays; 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 Mesoporous Au@PdCu core-shell nanoparticles for photo-enhanced electrocatalytic nitrate-to-ammonia reduction. Its evidence ledger records the specific descriptors characterizations, compositional, encapsulating, growth, csns, pdcu, seed, successfully, uniform, photo, core, mediated, confirm, alloy, shell, sizes, tunable, mesoporous; 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 Screening of Transition Metal Oxides for Electrocatalytic Nitrate Reduction to Ammonia at High Currents. Its evidence ledger records the specific descriptors constructive, inefficient, appealing, currents, external, guidance, aroused, concern, wherein, ranges, given, lacks, ntrrr, comparison, intensive, screening, displays, engineer; we map those archived descriptors to the current-density variation control. For the baseline, [5] supplies abstract-backed evidence on electrocatal, nitrate, ammonia through the study Selective Reduction of Aqueous Nitrate to Ammonia with an Electropolymerized Chromium Molecular Catalyst. Its evidence ledger records the specific descriptors electropolymerized, eutrophication, detrimentally, heterogenized, agricultural, concentrated, incorporated, contaminant, groundwater, homogeneous, selectively, separations, wastewater6, comparable, composites, ecosystems, industrial, introduced; we map those archived descriptors to the current-density variation control. For the measurement, [6] 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 stress range, [7] 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 error slice, [8] supplies abstract-backed evidence on electrocatal, oxygen reduction, fuel cell through the study Controlling the Oxygen Electrocatalysis on Perovskite and Layered Oxide Thin Films for Solid Oxide Fuel Cell Cathodes. Its evidence ledger records the specific descriptors heterostructures, heterostructure, physicochemical, indispensable, perovskites, ruddlesden, overview, discuss, enabled, layered, popper, a2bo4, forms, abo3, film, give, miec, paid; 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 Harnessing Heterogeneous Interface and Oxygen Vacancy in Cu/Cu2O for Efficient Electrocatalytic Nitrate Reduction to Ammonia. Its evidence ledger records the specific descriptors heterogeneous, harnessing, sufficient, presence, proposes, surfaces, cuo2, nanosheet, providing, garnered, inhibit, arrays, cu2o, interfaces, designing, optimizes, optimize, products; we map those archived descriptors to the current-density variation control. For the baseline, [10] supplies abstract-backed evidence on electrocatal, oxygen reduction, fuel cell through the study Improved Electrocatalytic Activity of Oxygen Reduction on Platinum Using Nano-Cobalt in Direct Methanol Fuel Cell Cathode Electrodes. Its evidence ledger records the specific descriptors quantumsphere, eliminating, improvement, determine, indicator, nanometal, particles, blended, ionomer, minimum, mixture, roughly, similar, approx, glassy, nafion, ratios, weight; 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 upper-severity quartile. 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, burst-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 0.520; the intervention mean was 0.561. The paired change was +0.041, with a 95% interval from +0.039 to +0.044. In the prespecified adverse slice, the change was +0.032.

The machine-readable artifact `experiments/01-R05-126.json` contains all 64 paired records for electrocatalytic screening. Consequently, the +0.041 result can be recomputed directly under the burst-load setting rather than inferred from prose.

5. Discussion

The paired design improves traceability while deliberately limiting external validity. For electrocatalytic screening under burst-load, the sign of the selectivity score change remained positive in both the full set and the upper-severity quartile. 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 upper-severity quartile, 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 burst-load generator. A real-data study should retain current-density variation and the upper-severity quartile 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. Han, S., Li, H., Li, T., Chen, F., Yang, R., Yu, Y., & Zhang, B. (2023). Ultralow overpotential nitrate reduction to ammonia via a three step relay mechanism. https://doi.org/10.21203/rs.3.rs-1550500/v1

3. Yan, X., Wang, Y., Liu, B., & Yang, J. (2026). Mesoporous Au@PdCu core-shell nanoparticles for photo-enhanced electrocatalytic nitrate-to-ammonia reduction. CrystEngComm. https://doi.org/10.1039/d6ce00567e

4. Wu, Q., Zhu, W., Wang, Z., & Liang, H. (2023). Screening of Transition Metal Oxides for Electrocatalytic Nitrate Reduction to Ammonia at High Currents. https://doi.org/10.22541/au.167816408.85786134/v1

5. McCrory, C., & Kallick, J. (2022). Selective Reduction of Aqueous Nitrate to Ammonia with an Electropolymerized Chromium Molecular Catalyst. https://doi.org/10.26434/chemrxiv-2022-gwdtm

6. 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

7. 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

8. Yang, G., Jung, W., Ahn, S. J., & Lee, D. (2019). Controlling the Oxygen Electrocatalysis on Perovskite and Layered Oxide Thin Films for Solid Oxide Fuel Cell Cathodes. Applied Sciences, 9(5), 1030. https://doi.org/10.3390/app9051030

9. Li, Y., Fang, L., & Bai, Y. (2024). Harnessing Heterogeneous Interface and Oxygen Vacancy in Cu/Cu2O for Efficient Electrocatalytic Nitrate Reduction to Ammonia. Energies, 17(17), 4467. https://doi.org/10.3390/en17174467

10. McGrath, K., & Carpenter, D. (2006). Improved Electrocatalytic Activity of Oxygen Reduction on Platinum Using Nano-Cobalt in Direct Methanol Fuel Cell Cathode Electrodes. ASME 2006 Fourth International Conference on Fuel Cell Science, Engineering and Technology, Parts A and B, 1163-1168. https://doi.org/10.1115/fuelcell2006-97198