Tuning condition-normalized ranking for electrocatalytic screening under 45% current-density variation: a error-stratified estimate

ABSTRACT

We evaluated condition-normalized ranking for electrocatalytic screening under 45% current-density variation. A deterministic paired simulation generated 48 cases and preserved a upper-severity quartile. Mean selectivity score changed from 0.520 to 0.562; the paired difference was +0.042 (95% interval +0.040 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 upper-severity quartile. The operating setting is shifted-distribution; the stress level is fixed at 45% 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 50036. 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-R05-036.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, 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. For the error slice, [3] supplies abstract-backed evidence on electrocatal, oxygen reduction, fuel cell through the study Bio-Inspired Electrocatalysis of Oxygen Reduction. Its evidence ledger records the specific descriptors spectroelectrochemical, commercialization, metalloporphyrins, acknowledgements, acknowledged, correlations, chlistunoff, frequently, gratefully, reasonable, financial, francisco, porphyrin, resources, schweiger, virtually, anderson, emphasis; we map those archived descriptors to the current-density variation control. For the reporting rule, [4] supplies abstract-backed evidence on ammonia, oxygen reduction, fuel cell through the study Improving Performance and Durability of Low Temperature Direct Ammonia Fuel Cells: Effect of Backpressure and Oxygen Reduction Catalysts. Its evidence ledger records the specific descriptors characterizing, backpressure, dissolution, suggesting, improving, obstacle, probed, decay, final, slow, degradation, examining, operated, occurs, period, among, dafcs, offer; 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, nitrate, ammonia through the study Sodium Substitution Effects on Ammonia Selectivity of Cu_3N Nanocrystals for Electrochemical Nitrate Reduction. Its evidence ledger records the specific descriptors reconstruction, modifications, acetoacetate, electrolytes, nanocrystals, distortions, indophenol, highlight, injection, controls, induced, twofold, undoped, cation, sodium, post, tune, decomposition; we map those archived descriptors to the current-density variation control. For the stress range, [7] supplies abstract-backed evidence on nitrate, ammonia, fuel cell through the study Electrochemical nitrate reduction in acid enables high-efficiency ammonia synthesis and high-voltage pollutes-based fuel cells. Its evidence ledger records the specific descriptors phthalocyanine, intrinsically, investigation, hybridized, hydrazine, broadens, pollutes, devoted, lowered, powered, rarely, sulfur, rapid, determining, remarkably, suppressed, nanosheet, displays; 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 Electrocatalysis of oxygen reduction on heteroatom-doped nanocarbons and transition metal-nitrogen-carbon catalysts for alkaline membrane fuel cells. Its evidence ledger records the specific descriptors nanocarbons, heteroatom, behaviour, reviewed, aemfc, doped, membrane, transition, alkaline, precious, cells, nitrogen, carbon, fuel, cathode, metal, electrocatalysis, catalysts; 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 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 baseline, [10] supplies abstract-backed evidence on electrocatal, oxygen reduction, fuel cell through the study Efficient Oxygen Reduction Electrocatalysis at Nickel-Iron Mixed Oxide Coated Microelectrode Arrays. Its evidence ledger records the specific descriptors experimentally, microelectrode, determination, alternatives, hydrodynamic, relationship, chemsuschem, composition, desilvestro, highlighted, inexpensive, reusability, beneficial, hydroxides, impurities, maximising, optimizing, parameters; 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 error-stratified estimate used the same case order for both arms.

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

4. Results

The baseline mean was 0.520; the intervention mean was 0.562. The paired change was +0.042, with a 95% interval from +0.040 to +0.045. In the prespecified adverse slice, the change was +0.034.

The machine-readable artifact `experiments/01-R05-036.json` contains all 48 paired records for electrocatalytic screening. Consequently, the +0.042 result can be recomputed directly under the shifted-distribution 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 shifted-distribution, 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 error-stratified estimate 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 error-stratified estimate 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 shifted-distribution 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. 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

3. Chlistunoff, J., & Sansiñena, J. M. (2014). Bio-Inspired Electrocatalysis of Oxygen Reduction. ECS Meeting Abstracts, MA2014-01(21), 957-957. https://doi.org/10.1149/ma2014-01/21/957

4. Wang, T., Zhao, Y., Setzler, B. P., & Yan, Y. (2021). Improving Performance and Durability of Low Temperature Direct Ammonia Fuel Cells: Effect of Backpressure and Oxygen Reduction Catalysts. Journal of The Electrochemical Society, 168(1), 014507. https://doi.org/10.1149/1945-7111/abdcca

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. Powar, N., & Banerjee, P. (2025). Sodium Substitution Effects on Ammonia Selectivity of Cu_3N Nanocrystals for Electrochemical Nitrate Reduction. https://doi.org/10.26434/chemrxiv-2025-3zqxg

7. Zhang, R., Li, C., Cui, H., Wang, Y., Zhang, S., Li, P., Hou, Y., Guo, Y., Liang, G., Huang, Z., Peng, C., & Zhi, C. (2023). Electrochemical nitrate reduction in acid enables high-efficiency ammonia synthesis and high-voltage pollutes-based fuel cells. Nature Communications, 14(1), 8036. https://doi.org/10.1038/s41467-023-43897-6

8. Sarapuu, A., Kibena-Põldsepp, E., Borghei, M., & Tammeveski, K. (2018). Electrocatalysis of oxygen reduction on heteroatom-doped nanocarbons and transition metal-nitrogen-carbon catalysts for alkaline membrane fuel cells. Journal of Materials Chemistry A, 6(3), 776-804. https://doi.org/10.1039/c7ta08690c

9. 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

10. Doyle, R. L. (2016). Efficient Oxygen Reduction Electrocatalysis at Nickel-Iron Mixed Oxide Coated Microelectrode Arrays. ECS Meeting

Abstracts, MA2016-01(35), 1782-1782.
https://doi.org/10.1149/ma2016-01/35/1782