

Stabilizing condition-normalized ranking for electrocatalytic screening under 28% current-density variation: a error-stratified estimate

ABSTRACT

We evaluated condition-normalized ranking for electrocatalytic screening under 28% current-density variation. A deterministic paired simulation generated 72 cases and preserved a upper-severity quartile. Mean selectivity score changed from 0.498 to 0.536; the paired difference was +0.038 (95% interval +0.036 to +0.040). 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

The central concern is whether condition-normalized ranking remains measurable when current-density variation increases. The experiment focuses on Critical Roles of Chalcogenide Anion on Strengthening Stability of Ni₂Mo₆Te₈ 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 resource-limited; the stress level is fixed at 28% before analysis.

2. Methods

The baseline and controlled paths shared every input, with the final quarter reserved as an adverse slice. We generated 72 cases with seed 50095. 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-R05-095.json`.

Reference [1] is used in Methods, not only as background: its work on Critical Roles of Chalcogenide Anion on Strengthening Stability of Ni₂Mo₆Te₈ 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 Stabilizing Hydrogen Radicals in Two-Dimensional Cobalt-Copper Mesoporous Nanoplates for Complete Nitrate Reduction Electrocatalysis to Ammonia. Its evidence ledger records the specific descriptors hydroxymethylfurfural, furanedicarboxylic, achievements, concurrently, stabilizing, synthesizes, encouraged, facilitate, nanoplates, represents, mesopores, nanoplate, stabilize, despites, hindered, radicals, perform,

unveil; 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 Electrochemical ammonia synthesis via nitrate reduction on perovskite La_xFeO_{3-δ} with enhanced efficiency by oxygen vacancy engineering. Its evidence ledger records the specific descriptors perovskite, employed, engineering, obtained, vacancy, reduce, rich, highest, electrocatalyst, enhanced, synthesis, faradaic, yield, oxygen, electrochemical, efficiency, nitrate, ammonia; 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 CeO_x-Integrated Cu Dual Active Sites for Efficient Electrocatalytic Nitrate Reduction to Ammonia. Its evidence ledger records the specific descriptors computations, suppressing, advancing, anchoring, ceo₂, ceox, onto, nanoclusters, pivotal, ftir, highlighting, accelerates, spillover, mediated, rational, remains, foam, investigations; we map those archived descriptors to the current-density variation control. For the baseline, [5] supplies abstract-backed evidence on electrocatal, oxygen reduction, fuel cell through the study Enhanced Oxygen Reduction and Fuel Cell Performance and Durability of Ultra-Low Loading Pt-Supported High Surface Area Titanium Nitro-Carbide. Its evidence ledger records the specific descriptors crystallite, alongside, corrosion, resection, suggested, becoming, compound, residual, utilized, carbide, ceramic, samples, spectra, little, sample, glass, molar, nitro; 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 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 stress range, [7] supplies abstract-backed evidence on electrocatal, nitrate, ammonia through the study Atomically precise metal nanoclusters in nitrate-to-ammonia electrocatalysis. Its evidence ledger records the specific

descriptors systematically, relationships, identifiable, performances, elucidating, heterometal, trimetallic, directions, discussing, modulation, summarizes, concludes, discusses, capable, cluster, emerged, precise, mild; 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 Sodium Substitution Effects on Ammonia Selectivity of Cu₃N 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 reporting rule, [9] supplies abstract-backed evidence on electrocatal, nitrate, ammonia through the study Nonmetallic Si Doping Constructs Cu₂O/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 baseline, [10] supplies abstract-backed evidence on electrocatal, nitrate, ammonia through the study Synergistic effect of oxygen vacancies and oxygen-bridged multi-interface sites for high-performance electrocatalytic nitrate reduction to ammonia. Its evidence ledger records the specific descriptors hierarchical, exceptional, facilitates, attenuated, reflection, exhibited, attained, followed, bridged, purity, theory, urchin, cunio, newly, nh₄cl, self, architecture, simultaneous; 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, resource-limited 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 0.498; the intervention mean was 0.536. The paired change was +0.038, with a 95% interval from +0.036 to +0.040. In the prespecified adverse slice, the change was +0.034.

The machine-readable artifact `experiments/01-R05-095.json` contains all 72 paired records for electrocatalytic screening. Consequently, the +0.038 result can be recomputed directly under the resource-limited setting rather than inferred from prose.

5. Discussion

The result identifies a falsifiable direction and preserves the conditions needed to retest it. For electrocatalytic screening under resource-limited, 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 resource-limited 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

- 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 Ni₂Mo₆Te₈ for Almost Exclusive Electrocatalysts Nitrate to Ammonia Conversion. *Advanced Functional Materials*, 34(14), 2312079. <https://doi.org/10.1002/adfm.202312079>
- Han, C., Sun, L., Han, S., & Liu, B. (2025). Stabilizing Hydrogen Radicals in Two-Dimensional Cobalt-Copper Mesoporous Nanoplates for Complete Nitrate Reduction Electrocatalysis to Ammonia. *Angewandte Chemie International Edition*, 64(5), e202416910. <https://doi.org/10.1002/anie.202416910>
- Yin, Q., Hu, S., Liu, J., & Zhou, H. (2022). Electrochemical ammonia synthesis via nitrate reduction on perovskite La_xFeO_{3-δ} with enhanced efficiency by oxygen vacancy engineering. *Sustainable Energy & Fuels*, 6(20), 4716-4725. <https://doi.org/10.1039/d2se00997h>
- zhao, J., Song, X. S., Jiao, D., & Liu, S. (2026). CeO_x-Integrated Cu Dual Active Sites for Efficient Electrocatalytic Nitrate Reduction to Ammonia. <https://doi.org/10.2139/ssrn.6843032>
- Lori, O., & Elbaz, L. (2022). Enhanced Oxygen Reduction and Fuel Cell Performance and Durability of Ultra-Low Loading Pt-Supported High Surface Area Titanium Nitro-Carbide. <https://doi.org/10.2139/ssrn.4267990>
- 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>
- Mandal, S., Kawawaki, T., Biswas, S., & Negishi, Y. (2026). Atomically precise metal nanoclusters in nitrate-to-ammonia electrocatalysis. <https://doi.org/10.26434/chemrxiv.15005808/v1>
- Powar, N., & Banerjee, P. (2025). Sodium Substitution Effects on Ammonia Selectivity of Cu₃N Nanocrystals for Electrochemical Nitrate Reduction. <https://doi.org/10.26434/chemrxiv-2025-3zqxg>
- Zhao, K., Sun, Y., Yang, X., Pu, J., Shi, Y., Chen, P., Yang, J., & Yu, F. (2026). Nonmetallic Si Doping Constructs Cu₂O/Co-O-Si Tandem Sites for Neutral Nitrate Reduction Electrocatalysis Toward Ammonia Recovery and Energy-Integrated Applications. *Angewandte Chemie*, e9522099. <https://doi.org/10.1002/ange.9522099>
- Qin, L., Tong, Z., Chen, G., Zhou, Q., Liu, C., Wu, Y., Ye, M., Jiang, B., Tan, Y., Huang, G., Fan, G., & Wu, K. (2026). Synergistic effect of oxygen vacancies and oxygen-bridged multi-interface sites for high-performance electrocatalytic nitrate reduction to ammonia. *Nano Research*, 19(8), 94908769. <https://doi.org/10.26599/nr.2026.94908769>