Calibrating condition-normalized ranking for electrocatalytic screening under 33% current-density variation: a blocked comparison

ABSTRACT

We evaluated condition-normalized ranking for electrocatalytic screening under 33% current-density variation. A deterministic paired simulation generated 56 cases and preserved a upper-severity quartile. Mean selectivity score changed from 0.502 to 0.539; the paired difference was +0.037 (95% interval +0.035 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

Performance averages can obscure whether current-density variation changes the reliability of electrocatalytic screening. 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 sparse-observation; the stress level is fixed at 33% before analysis.

2. Methods

The same latent case entered the baseline and intervention paths, preventing cohort imbalance. We generated 56 cases with seed 50065. 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-R05-065.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 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. For the error slice, [3] supplies abstract-backed evidence on electrocatal, oxygen reduction, fuel cell through the study Low-Platinum Electrocatalysts for the Oxygen Reduction Reaction at Fuel Cell Cathodes. Its evidence ledger records the specific descriptors demonstration, spectrometry, transmission, christopher, inductively, stamenkovic, thicknesses, department, leveraging, mechanical, microscopy, rigorously, volkswagen, chemistry, currently, jousselme, tsiakaras, wolfsburg; 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 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 baseline, [5] 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 measurement, [6] supplies abstract-backed evidence on electrocatal, nitrate, ammonia through the study CeOx-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 stress range, [7] supplies abstract-backed evidence on electrocatal, nitrate, ammonia through the study Photoelectrochemical Nitrate Reduction to Ammonia: Materials, Methods, and Metrics. Its evidence ledger records the specific descriptors photoelectrochemically, photoelectrochemical, recommendations, standardisation, lightabsorbing, architectures, methodologies, thermodynamic, underpinning, contributor, accelerate, analytical, critically, feedstock, summarise, fixation, clarify, metrics; 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 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 reporting rule, [9] 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, a2b04, forms, ab03, film, give, miec, paid; 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 Oxygen Reduction Electrocatalysts in Proton Exchange Membrane Fuel Cells. Its evidence ledger records the specific descriptors precombustion, accelerating, combustion, conclusion, researcher, seperation, addressed, assessing, enhancing, molecules, objective, principal, carrying, covering, previous, decides, demands, favored; 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 blocked comparison used the same case order for both arms.

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

4. Results

The baseline mean was 0.502; the intervention mean was 0.539. The paired change was +0.037, with a 95% interval from +0.035 to +0.040. In the prespecified adverse slice, the change was +0.034.

The machine-readable artifact `experiments/01-R05-065.json` contains all 56 paired records for electrocatalytic screening. Consequently, the +0.037 result can be recomputed directly under the sparse-observation setting rather than inferred from prose.

5. Discussion

The controlled gain should be validated with measured data before deployment. For electrocatalytic screening under sparse-observation, 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 blocked comparison 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 blocked comparison 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 sparse-observation 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.

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