QuantumNovelty Review Showcase

Paper audit Generative flow-based warm start of the variational quantum eigensolver (arXiv:2507.01726)

Generated by the QuantumNovelty paper-audit pipeline

June 2026

Project	QuantumNovelty (QN) — audit-and-falsify framework for quantum-computing research
Repository	https://github.com/boltzmannentropy/QuantumNovelty
Author	Shlomo Kashani (QNeura.ai)
LLM backend	Claude Code CLI (`2.1.1 (Claude Code)`)
Model snapshots used	`claude-haiku-4-5-20251001` `claude-opus-4-5-20251101`
Report generated	2026-06-10 23:18 by `build_reviews.py`

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1 Papers under review

Tag	Paper	Venue	arXiv
`flowvqe`	Generative flow-based warm start of the variational quantum eigensolver Hang Zou, Martin Rahm, Anton Frisk Kockum, Simon Olsson	npj Quantum Information (2025)	2507.01726

2 Token + cost ledger

Every LLM call records the model snapshot ID, exact input/output token counts, and USD cost from the Claude CLI's JSON envelope.

Paper	Stage	Input tk	Output tk	Cost ($)	Elapsed (s)
flowvqe	Deep-research review	1	1,318	$0.2581	38.0
flowvqe	Reviewer panel 5 voices	1	4,646	$0.3421	109.5
flowvqe	Logical-fallacy report	1	2,863	$0.2955	52.8
flowvqe	Stage-6 CQE narrative	2	1,180	$0.0721	31.7
flowvqe total		**5**	**10,007**	**$0.9678**	**232.0**
Grand total		**5**	**10,007**	**$0.9678**	**232.0**

3 Verdict summary

Paper	Panel score	EIC verdict	CQE composite
`flowvqe`	6.0/10	major-revisions	23/100

Panel score is the mean of the five voices' *Verdict: N/10* scores; the EIC verdict comes from the vote table; the CQE composite is the geometric mean of the six process-quality dimensions.

4 flowvqe — *Generative flow-based warm start of the variational quantum eigensolver*

Hang Zou, Martin Rahm, Anton Frisk Kockum, Simon Olsson arXiv:2507.01726 npj Quantum Information (2025)

4.1 flowvqe — Deep-research review

Model: `claude-haiku-4-5-20251001` · 1,318 output tokens · 38.0 s

4.1.1 1. One-paragraph summary of what the paper claims

The paper introduces Flow-VQE, a framework that uses conditional normalizing flows to generate high-quality variational parameters for the Variational Quantum Eigensolver (VQE). The authors claim that by embedding a generative model into the VQE optimization loop via preference-based training, Flow-VQE enables gradient-free optimization and provides a systematic approach for parameter transfer across related molecular systems. Through numerical simulations on H, HO, NH, and CH, they report that Flow-VQE achieves computational accuracy with fewer circuit evaluations than baseline optimizers (improvements ranging from modest to over two orders of magnitude), and when used for warm-starting, accelerates subsequent fine-tuning by up to 50-fold compared to Hartree-Fock initialization. The total training overhead is claimed to be no greater than optimizing five molecules by conventional methods.

4.1.2 2. Audit-and-falsify checklist

Criterion	Verdict	Evidence
Augmented baseline catalog	PARTIAL	The paper compares against GD, Adam, and QNSPSA, which are standard VQE optimizers, but does not benchmark against recent ML-based warm-start methods (e.g., meta-learning approaches [40-44], supervised learning [32,33], or other generative approaches [34,35]) that they cite in the introduction.
Strict-domination comparator	FAIL	Claims like "up to two orders of magnitude" and "50-fold acceleration" are stated without specifying calibrated tolerances (_abs, _rel); Figures 2 and 4 show bar plots without error bars or statistical uncertainty quantification on the circuit evaluation counts.
Recompute-from-raw	FAIL	No raw numerical tables are provided in the paper or supplementary material; ratios and improvement factors cannot be independently verified from tabulated source data (Table I provides post-training comparison but not the raw data underlying Figures 2-4).
Wilson 95% CIs	FAIL	No confidence intervals are reported on any results; particularly concerning for small-sample comparisons (e.g., 6 geometries for HO, 8 for H) and the batch size B=2 sampling regime where statistical fluctuations would be substantial.
Cross-LLM falsifiability	NOT-APPLICABLE	This paper does not use an LLM-in-the-loop method; the generative model is a normalizing flow trained via preference optimization, not a language model.

Criterion	Verdict	Evidence
Honest negatives	PARTIAL	The paper acknowledges limitations in Section VI (reduced diversity over training, potential loss of exploration, less precision than gradient-based methods in smooth landscapes), but does not include a dedicated Failure Modes section showing specific cases where Flow-VQE failed to improve over baselines or failed to converge.
Simulator precision floor	FAIL	No mention of float64 vs complex64 precision; all experiments use PennyLane state-vector simulations without specifying numerical precision, which is relevant given the "computational accuracy" threshold of 1.6Œ10ş Hartree.
Auditable claims	FAIL	No audit_claims.py or equivalent script is provided; no mention of code/data availability in the paper body (required statements for npj Quantum Information are absent from this preprint version).

4.1.3 3. Overall assessment

This paper presents a creative and potentially impactful idea—using normalizing flows with preference-based training to warm-start VQE—but the empirical validation falls significantly short of the rigour expected for claims of "up to two orders of magnitude" improvement. The absence of error bars, confidence intervals, or statistical tests on performance metrics undermines confidence in the reported speedups. The baseline comparisons exclude the very ML-based methods the paper positions itself against in the introduction. No raw data tables or reproducibility scripts are provided, making independent verification impossible. The paper would likely not survive a strict reviewer-mode audit in its current form: the methodology is interesting but the evidence is presented at display precision without uncertainty quantification, and several required statements for the target journal (Code Availability, Data Availability) are missing from the preprint.

Research rigour score: 4/10

4.1.4 4. Three highest-leverage improvements

1. **Add statistical uncertainty to all quantitative claims**: Report Wilson 95% confidence intervals or bootstrap CIs for circuit-evaluation counts, especially given the small number of molecular geometries (6-8 per system). Run multiple random seeds for all methods and report mean ś std across seeds. The "50-fold" and "two orders of magnitude" claims should be converted to ratios with confidence bounds (e.g., "27Œ [95% CI: 18-41]").

2. **Benchmark against ML-based warm-start methods**: The paper cites meta-learning [40-44], supervised learning [32,33], and generative approaches [34,35] but only compares against traditional optimizers. Include at least one ML-based warm-start baseline (e.g., FLIP [42] or a supervised neural-network initializer) to demonstrate strict domination over current published methods, not just textbook baselines.

3. **Provide auditable artifacts and raw data**: Create an `audit_claims.py` (or equivalent) that derives every numerical claim (improvement ratios, circuit counts, energy errors) from on-disk JSON/CSV files. Include a Data Availability and Code Availability statement with a permanent repository link. Specify the numerical precision (float64/complex64) used in all simulations and provide the exact random seeds for reproducibility.

4.2 flowvqe — Reviewer panel 5 voices

Model: `claude-haiku-4-5-20251001` · 4,646 output tokens · 109.5 s

Peer Review Panel: Flow-VQE Manuscript

4.2.1 Voice 1 — Reviewer 1 (Physics correctness)

The manuscript presents a methodologically sound approach to variational quantum eigensolver optimization through normalizing flows. The Hamiltonian construction follows standard procedures: Jordan-Wigner transformation for fermion-to-qubit mapping, active space selections that are physically reasonable ((4e,4o) for H, (6e,5o) for HO, (6e,6o) for NH and CH), and appropriate basis sets (STO-3G for the larger molecules, cc-pVDZ for H). The choice of Jordan-Wigner over Bravyi-Kitaev or parity mappings is not justified but is defensible given the modest qubit counts (5-12 qubits). The Z symmetry tapering applied to H is correctly implemented and reduces the qubit count from 8 to 5, which is standard practice.

The Hartree-Fock reference initialization strategy is well-motivated. The authors correctly note that HF typically recovers >99.5% of total electronic energy for small closed-shell molecules, making the remaining correlation energy the critical optimization target. The ansatz choices are appropriate: the hardware-efficient RY-linear ansatz for H and Givens-based singles and doubles (GSD) for the other molecules. The GSD ansatz preserves particle number and spin symmetry by construction, which is crucial for chemical accuracy. However, the manuscript does not discuss the expressibility limits of these ansätze in relation to the active spaces chosen—particularly whether the GSD ansatz with 54-117 parameters can capture the full correlation energy within the selected active spaces.

One concern is the absence of discussion regarding numerical precision. The simulations are performed via PennyLane state-vector simulation, but the manuscript does not specify whether complex128 or complex64 precision was used. For stretched geometries where strong correlation effects dominate (e.g., H at 2.6 Å or HO at 1.9 Å), numerical precision can significantly affect the computed energies, particularly when comparing against "exact diagonalization at the same level of theory." The claimed computational accuracy threshold of 1.6Œ10ş Hartree (~1 kcal/mol) is chemically meaningful, but the authors should verify that numerical artifacts do not contaminate their comparisons at this precision level.

The treatment of stretched bond regions deserves additional scrutiny. The authors acknowledge that "energy errors increase in stretched bond-length regions due to strong correlation effects and the limited expressivity of the employed ansätze." This is physically correct, but the manuscript would benefit from quantifying the multireference character (e.g., via T1 diagnostic or natural orbital occupation numbers) to distinguish between ansatz limitations and Flow-VQE performance. Additionally, the equilibrium geometries and bond stretching ranges are reasonable for benchmarking, but the ammonia inversion coordinate and benzene C-H stretch represent different classes of nuclear motion that test different aspects of the PES—this diversity is a strength, but the physical rationale for these choices could be made more explicit.

Questions for Authors: 1. What numerical precision (complex64 vs complex128) was used in the state-vector simulations, and have you verified that precision artifacts do not affect comparisons at the 1.6Œ10ş Hartree threshold? 2. Can you provide multireference diagnostics (T1 amplitudes or natural orbital occupations) for the stretched geometries to distinguish ansatz expressibility limitations from optimization performance? 3. Why was Jordan-Wigner chosen over Bravyi-Kitaev, given that BK can reduce circuit depth for certain ansätze? 4. For the GSD ansatz, have you verified that 54-117 parameters are sufficient to reach the FCI limit within your active spaces?

Verdict: 7/10 — Minor Revisions

4.2.2 Voice 2 — Reviewer 2 (Algorithmic novelty)

The core algorithmic contribution—using conditional normalizing flows trained via preference-based optimization to generate VQE parameters—represents a meaningful advance over prior work, though the novelty claims require careful contextualization. The manuscript correctly identifies key limitations of existing approaches: gradient-based methods incur O(d) overhead per iteration, gradient-free methods scale poorly with dimensionality, and conventional parameter transfer relies on geometric proximity heuristics. Flow-VQE addresses these through a learned conditional prior that can generalize across chemical space.

Comparing against recent literature (2023-2025), several closely related works warrant discussion. Rudolph et al. (Nat. Commun. 2023, Ref. [25]) demonstrated tensor-network pretraining for parameterized quantum

circuits, achieving similar goals of informed initialization. The manuscript does cite this but does not provide direct numerical comparison. More critically, Nakaji et al. (arXiv 2401.09253, Ref. [80]) introduced the Generative Quantum Eigensolver (GQE), which generates entire quantum circuits rather than just parameters—a more ambitious scope that subsumes Flow-VQE's approach. The authors acknowledge this in Section VI as future work but should more directly address how Flow-VQE relates to GQE's published results. Additionally, Chang et al. (arXiv 2505.10842, Ref. [44]) propose LSTM-based parameter prediction specifically for VQE, published after the apparent submission of this work but representing convergent thinking that affects novelty assessment.

The preference-based optimization scheme (Section III.C) is the most novel technical contribution. Drawing from RLHF methods in language models (DPO, Ref. [68]), the authors replace high-variance policy gradients with pairwise comparisons and elite buffer maintenance. This is clever and well-motivated: the observation that "chemically meaningful energy differences translate to extremely weak learning signals" (Section III.B.1) is correct and explains why vanilla REINFORCE would struggle. However, the connection to established preference learning theory is somewhat superficial—the authors do not discuss the implicit reward model induced by their approach or how it relates to Bradley-Terry preferences.

Regarding claimed performance ratios, the headline numbers ("up to two orders of magnitude fewer circuit evaluations," "50-fold acceleration") require scrutiny. Examining Figure 2, the two-orders-of-magnitude claim appears to derive from comparing Flow-VQE-S against gradient descent at specific bond lengths (e.g., HO at 1.8 Å shows ~10š improvement). However, the appropriate baseline comparison should be against Adam with properly tuned learning rates, where improvements are 2-5Œ according to the authors' own text. The 50-fold warm-start acceleration (Table I) occurs at learning rate =0.001, which is unrealistically conservative for standard VQE—practitioners typically use [0.01, 0.1]. At =0.02, the improvement is ~27Œ for HO and ~11Œ for H, which are still impressive but more modest. These nuances should be foregrounded rather than buried.

Questions for Authors: 1. Can you provide direct numerical comparison against tensor-network pretraining (Rudolph et al.) and/or GQE (Nakaji et al.) on overlapping benchmark molecules? 2. What implicit reward model does your preference-based training induce, and how does it relate to Bradley-Terry or Plackett-Luce models? 3. Why were baseline comparisons performed at =0.02 rather than grid-searching for optimal baseline learning rates, given that your headline improvements depend on baseline performance?

Verdict: 6/10 — Major Revisions

4.2.3 Voice 3 — Reviewer 3 (Empirical evidence)

The experimental methodology presents several concerns regarding statistical rigor, reproducibility, and completeness of ablations. While the numerical results are promising, the empirical evidence does not meet the standards expected for a high-profile computational quantum chemistry publication.

The most significant gap is the absence of uncertainty quantification. All reported circuit evaluation counts and energy errors are point estimates without confidence intervals or multi-seed variance. Given the stochastic nature of both the normalizing flow sampling and the preference-based training, results should be reported over multiple random seeds (n5 is typical). For example, the claim that "Flow-VQE-S achieves approximately a two- to five-fold reduction" over Adam lacks error bars—does this range reflect variation across molecules, or could it also reflect run-to-run variance that would widen the comparison? Table I reports final energy errors to 4 significant figures (e.g., 5.932Œ10 Hartree), but without standard deviations, these precision claims are unverifiable.

The ablation study is incomplete. The authors introduce several design choices—Gaussianization flows versus alternative architectures, 7-20 flow layers, buffer size M=2, batch size B=2, Gaussian noise regularization (š=0.001), and linear Hamiltonian embeddings—but do not systematically ablate their contributions. Section VI acknowledges that "Flow-VQE introduces some additional hyperparameters... which may require more empirical tuning," but the reader is left without guidance on which choices are critical. Particularly concerning is the elite buffer size M=2: with only two samples retained per configuration, the training could be highly sensitive to early lucky draws. An ablation varying M{1, 2, 5, 10} would clarify whether the method is robust.

The comparison against baselines raises methodological questions. The authors compare Flow-VQE against GD, Adam, and QNSPSA with fixed hyperparameters, but hyperparameter optimization is standard practice for baseline comparisons. The statement "All baseline optimizers use a learning rate of =0.02" in Figure 2 suggests baselines were not individually tuned, potentially handicapping them. Additionally, the QNSPSA comparison is

welcome (as a gradient-free method), but the manuscript does not include other recent gradient-free approaches such as COBYLA, Nelder-Mead, or evolutionary strategies that are commonly used in VQE literature.

Reproducibility infrastructure is not adequately described. The manuscript mentions "state-vector simulation experiments" using PennyLane and OpenFermion but does not provide: (a) version numbers for software dependencies, (b) hardware specifications for classical computation, (c) wall-clock training times, or (d) code/data availability statements beyond acknowledging NAISS computational resources. For a method whose practical utility depends on the classical overhead remaining "easily tractable with modern machine learning techniques," timing data would strengthen the claims. The required npj Quantum Information statements (Code Availability, Data Availability) appear to be missing from the current draft.

Questions for Authors: 1. Can you report multi-seed variance (n5) for the key comparisons in Figures 2-4 and Table I? 2. What ablations can you provide for buffer size M, batch size B, flow depth, and regularization noise? 3. Will code and data be released upon publication, and at what URL? 4. What are the wall-clock training times for Flow-VQE-S and Flow-VQE-M on a specified hardware configuration?

Verdict: 5/10 — Major Revisions

4.2.4 Voice 4 — Devil's Advocate

This manuscript exemplifies a troubling trend in quantum computing: impressive-sounding improvements over carefully chosen baselines that dissolve under scrutiny. Let me enumerate the fundamental problems that my fellow reviewers have been too generous about.

The baseline comparisons are rigged. The entire narrative hinges on comparing against gradient descent, an optimizer no serious VQE practitioner would use for production work. The authors bury the admission that "Flow-VQE-S achieves approximately a two- to five-fold reduction" over Adam—this is the *only* meaningful comparison, and 2-5Œ improvement is incremental, not transformative. The "two orders of magnitude" headline claim requires comparing against raw GD at =0.02 without momentum, which is a strawman. Furthermore, baseline optimizers were run with identical learning rates rather than individually tuned, while Flow-VQE's hyperparameters (learning rate, weight decay, flow depth, buffer size, batch size, noise variance) were presumably chosen via undocumented empirical search. This asymmetry invalidates the entire quantitative comparison.

The method cannot scale. The authors test on systems with 5-12 qubits and 54-117 parameters. Modern quantum chemistry requires hundreds to thousands of qubits. Section VI's optimistic claim that "the classical overhead in modern normalizing-flow architectures scales linearly in d" ignores the elephant in the room: flow models require O(d) samples to estimate the target distribution in d dimensions, and preference-based training with buffer size M=2 cannot possibly capture a meaningful distribution over 10,000+ parameters. The authors' own Figure 6 shows extensive stagnation plateaus even at d100—these will become impassable walls at chemically relevant scales. The comparison against parameter transfer (Figure 4) shows Flow-VQE-M only marginally outperforming PT, which requires no neural network overhead whatsoever.

The experimental design hides failures. Why are only four molecules tested? Why these specific geometric distortions? The authors test HO bond stretching, H linear chain stretching, NH inversion, and CH C-H stretch—but conspicuously absent are: (a) molecules with transition metals, (b) open-shell systems, (c) excited states, (d) strongly correlated systems beyond stretched bonds, and (e) any molecule requiring >12 qubits. The selection bias suggests the authors tried other systems and failed. The manuscript contains no honest negatives, no failure modes section, and no discussion of when Flow-VQE underperforms baselines. Figure 2(b) shows Flow-VQE-S *losing* to Adam at H 0.6 Å—this is mentioned in passing but not analyzed. A rigorous empirical study would characterize the conditions under which the method fails.

The novelty is overstated. The core idea—use generative models to propose VQE parameters—appears in multiple prior works: Ceroni et al. (Ref. [34], 2023), Zhang et al. (Ref. [35], 2025), and Nakaji et al. (Ref. [80], 2024). The preference-based training draws directly from DPO in language models without significant adaptation for quantum settings. The Gaussianization flow architecture is off-the-shelf (Meng et al., AISTATS 2020). The conditional embedding via Hamiltonian coefficients is straightforward. Stripping away the quantum framing, this is a routine application of conditional generative modeling to a black-box optimization problem—technically competent but not meeting the novelty bar for a flagship publication.

The required journal elements are missing. npj Quantum Information mandates Author Contributions, Competing Interests, Data Availability, and Code Availability statements. None appear in this draft. The

Methods section is scattered throughout rather than consolidated at the end per Nature/npj conventions. The abstract (currently 248 words) barely meets the 250-word limit. These are not fatal flaws but indicate either carelessness or unfamiliarity with the target venue.

Recommendation: Reject. The contributions do not justify publication in npj Quantum Information. The method shows modest improvements over properly chosen baselines, cannot scale to relevant system sizes, lacks statistical rigor, and does not advance the field beyond concurrent/prior work. The manuscript may be suitable for a computational chemistry venue after substantial revision.

4.2.5 Voice 5 — Editor-in-Chief synthesis

Having carefully considered all four reviews, I observe substantial disagreement regarding the manuscript's merits. Reviewer 1 finds the physics sound with minor concerns about numerical precision and ansatz expressibility. Reviewer 2 identifies legitimate novelty in the preference-based training scheme but requests stronger baseline comparisons and engagement with concurrent work. Reviewer 3 raises serious methodological concerns about statistical rigor and reproducibility that must be addressed. The Devil's Advocate presents the strongest case for rejection, emphasizing baseline selection bias, scalability limitations, and missing journal requirements.

Let me address the Devil's Advocate's critiques specifically, as they represent the highest bar the authors must clear. The baseline comparison criticism has merit: comparing against GD is indeed uninformative, and the Adam comparison should be the primary benchmark. However, the 2-5Œ improvement over Adam, combined with the generative warm-start capability (Table I), does represent meaningful practical utility—especially for practitioners who must optimize many related molecular configurations. The scalability criticism is fair but applies to essentially all NISQ algorithm papers; the authors appropriately scope their claims to near-term devices. The charge of hidden failures is partially addressed by the H 0.6 Å result where Flow-VQE underperforms, though I agree a dedicated failure analysis would strengthen the work. The novelty critique is the most serious: the manuscript must better differentiate from Nakaji et al. (GQE) and demonstrate why parameter-space generation offers advantages over circuit-space generation.

The statistical concerns raised by Reviewer 3 are non-negotiable for publication. Single-seed results without confidence intervals are insufficient for empirical claims. The missing Data/Code Availability statements violate npj QI policy and must be added. The incomplete ablation study leaves readers unable to assess which design choices are essential versus incidental.

Regarding the physics and chemistry (Reviewer 1), the concerns are addressable through clarifications rather than new experiments. The algorithmic novelty (Reviewer 2) requires engagement with concurrent literature but does not fundamentally undermine the contribution. The preference-based training adapted from RLHF to quantum chemistry contexts is a genuine methodological contribution, even if the components are individually known.

Final Verdict: Major Revisions

The manuscript presents a technically sound method with meaningful practical utility for VQE optimization across molecular configurations. However, the current presentation suffers from inflated claims relative to appropriate baselines, inadequate statistical rigor, missing journal-required elements, and insufficient differentiation from concurrent work. Acceptance is possible after substantial revision.

Must-fix items before resubmission (ordered by severity):

1. **Add multi-seed variance reporting** (n5) for all quantitative comparisons, including Figures 2-4 and Table I. Report 95% confidence intervals or standard deviations.

2. **Include Code and Data Availability statements** per npj QI requirements, with repository URLs and DOIs where applicable.

3. **Revise headline claims** to foreground Adam comparisons (2-5Œ improvement) rather than GD comparisons (100Œ). Move GD results to supplementary material or present as secondary.

4. **Add direct comparison with GQE** (Nakaji et al.) or explicitly justify why parameter-space generation is preferable to circuit-space generation for the tested molecules.

5. **Provide ablation study** for buffer size M, flow depth, and regularization noise, minimally as supplementary material.

6. **Consolidate Methods section** at the end of the manuscript per Nature/npj conventions, and add required Author Contributions and Competing Interests statements.

7. **Specify numerical precision** (complex64/128) and verify that precision artifacts do not affect comparisons at the 1.6 mHa threshold.

8. **Add failure mode analysis** discussing conditions under which Flow-VQE underperforms baselines, expanding on the H 0.6 Å observation.

4.2.6 Vote table

Voice	Recommendation	Confidence 1-10
Reviewer 1	Minor Revisions	7
Reviewer 2	Major Revisions	6
Reviewer 3	Major Revisions	8
Devil's Advocate	Reject	7
Editor-in-Chief	Major Revisions	8

4.3 flowvqe — Logical-fallacy report

Model: `claude-haiku-4-5-20251001` · 2,863 output tokens · 52.8 s

I'll carefully analyze this quantum computing manuscript for logical fallacies using the provided taxonomy, focusing on findings with severity at or above **medium**.

Fallacy: cherry-picked-baseline **Severity:** high **Location:** Section I (Introduction) and Section V.A (Single-molecule optimization), Figure 2 **Evidence:** "We compare Flow-VQE to a number of standard benchmarks through numerical simulations… We find that Flow-VQE outperforms baseline optimization algorithms" and comparing against "gradient descent (GD), quantum natural-gradient simultaneous perturbation stochastic approximation (QNSPSA), Adam" **Why it's the fallacy:** The paper compares against generic optimization algorithms (GD, Adam, QNSPSA) but omits comparison with other published warm-start and ML-based VQE initialization methods that they explicitly cite as prior work (references [32-44]), including supervised learning approaches, meta-learning frameworks, and other generative modeling methods. For instance, they cite methods like FLIP [42] and meta-VQE [41] but don't benchmark against them on the same molecular systems. **Suggested fix:** Include direct numerical comparisons with at least one or two of the most relevant published warm-start methods (e.g., the supervised learning approaches from [32-33] or the meta-learning methods from [40-44]) on the same Hamiltonians, or explicitly state why such comparisons were not feasible and acknowledge this as a limitation.

Fallacy: conflated-regimes **Severity:** high **Location:** Section I (Introduction), Section VI (Limitations and Future Work) **Evidence:** "While the numerical experiments reported here extend only to 12-qubit active spaces and 117 variational parameters, several features of Flow-VQE promise broad quantum-resource savings, even when scaling to larger molecules." **Why it's the fallacy:** The paper extrapolates from small Hamiltonians (5-12 qubits, up to 117 parameters) to claims about larger systems without empirical validation. The claim that advantages will persist at scale is speculative, especially given that barren plateaus and optimization landscape complexity scale non-trivially with system size. The paper acknowledges this only partially in limitations but still makes forward-looking claims about scalability. **Suggested fix:** Temper scalability claims with explicit caveats. Replace "promise broad quantum-resource savings" with "may potentially offer resource savings pending empirical validation at larger scales" and acknowledge that the scaling behavior of the normalizing flow approach with qubit count remains uncharacterized.

Fallacy: hasty-generalization **Severity:** medium **Location:** Section V.C (Estimate of cost advantage) **Evidence:** "For NH3, standard VQE requires an average of CVQE = 5,265 circuit evaluations per test point... These estimates are instance-dependent and not intended as universal benchmarks, but they illustrate the practical advantages of Flow-VQE-M" **Why it's the fallacy:** The cost advantage analysis is based on only two molecules (NH3 and C6H6) with very limited training configurations (4 configurations each). The paper then uses these narrow results to draw broader conclusions about the method's advantages, despite acknowledging the estimates are "instance-dependent." **Suggested fix:** Explicitly state that the cost advantage calculations are illustrative examples from a narrow test set, not generalizable predictions. Add language such as: "These results demonstrate potential advantages in specific cases but should not be extrapolated to other molecular systems without further validation."

Fallacy: active-space-handwave **Severity:** medium **Location:** Section IV.A.1 (Electronic structure modeling) and Section VII (Conclusion) **Evidence:** "For active-space selections, we perform them to manage computational complexity while preserving essential electronic structure features: (4e, 4o) for H4, (6e, 5o) for H2O, (6e, 6o) for NH3, and (6e, 6o) for C6H6" combined with conclusion claims that "Flow-VQE can become a pragmatic and versatile paradigm" **Why it's the fallacy:** The paper uses small, carefully selected active spaces but claims generalization without running on larger or different active space selections. The choice of active spaces is not justified beyond "managing computational complexity," and there's no evidence the method would work for larger active spaces that would be needed for chemically meaningful calculations on these molecules. **Suggested fix:** Add explicit justification for why these specific active spaces were chosen and acknowledge that performance on larger, more chemically realistic active spaces remains untested. Include a statement like: "The active spaces used here are minimal and primarily serve as proof-of-concept; extension to larger active spaces required for chemical accuracy remains to be demonstrated."

Fallacy: hardware-irrelevant-comparison **Severity:** medium **Location:** Section IV (Numerical Simulations), throughout **Evidence:** "We empirically validate Flow-VQE through state-vector simulation experiments on various quantum chemical systems" and "We adopt the number of quantum circuit evaluations, independent of measurement shot counts, as the primary performance metric" **Why it's the fallacy:** All experiments are performed on ideal state-vector simulators without noise calibration or hardware validation. The paper claims the method is designed for "near-term quantum devices" and NISQ hardware, but provides no evidence of performance under realistic noise conditions. Circuit evaluation counts on simulators don't translate directly to hardware performance where noise accumulates. **Suggested fix:** Either include noisy simulations with realistic noise models, or clearly caveat that all results are for ideal simulators and that hardware validation is required before claims about NISQ utility can be made. Add explicit text: "All experiments were conducted under ideal noiseless conditions; performance under realistic hardware noise remains to be characterized."

Fallacy: asymptotic-only-claim **Severity:** medium **Location:** Section VI (Limitations and Future Work) **Evidence:** "On the classical side, the classical overhead in modern normalizing-flow architectures scales linearly in d, keeping training and inference practical even as d reaches the tens of thousands" **Why it's the fallacy:** The paper claims linear scaling to "tens of thousands" of parameters but only demonstrates results up to d=117 parameters. This asymptotic claim about classical overhead is not validated empirically in the presented work. **Suggested fix:** Either remove the claim about scaling to tens of thousands of parameters, or explicitly note this is a theoretical expectation that has not been validated: "While normalizing flow architectures theoretically scale linearly in d, we have only validated this up to d=117 in the present work."

Fallacy: unit-inflation **Severity:** medium **Location:** Section I (Abstract), Section V (Results) **Evidence:** "improvements range from modest to more than two orders of magnitude" and "up to 50-fold compared with

Hartree–Fock initialization" **Why it's the fallacy:** The paper presents maximum improvements ("up to," "more than two orders of magnitude") rather than typical or median improvements. The most dramatic improvements (50-fold, 100x) occur at specific learning rates (=0.001) or extreme bond lengths that may not represent typical use cases. The "two orders of magnitude" claim appears to come from outlier configurations. **Suggested fix:** Report median or geometric mean improvements alongside maximum improvements. Replace "up to 50-fold" with "improvements ranging from X-fold to 50-fold (median: Y-fold)" and clarify that the most dramatic improvements occur under specific conditions.

4.4 flowvqe — Stage-6 CQE narrative

Model: `claude-opus-4-5-20251101` · 1,180 output tokens · 31.7 s

Process Summary: QuantumNovelty Run Evaluation

4.4.1 Composite Verdict

The composite score of **23/100** places this run firmly in the "Critical Deficiencies" tier. On the standard 1-100 scale, scores below 30 indicate a run that failed to produce the fundamental artifacts required for a credible scientific claim. This is not a borderline result—it represents a systematic failure across nearly all evaluation dimensions.

A geometric mean of 23 from six dimensions means no single strong dimension could compensate for the others. The multiplicative nature of the composite punishes runs where any dimension collapses toward zero, and here we see scores of 8, 20, 27, 30, 30, and 40. The lowest scores drag the composite down irreversibly. This run produced neither the baseline comparisons nor the verification artifacts that would allow anyone—including the original researchers—to assess whether the results mean anything.

4.4.2 Strongest Dimension: Communication (40)

Communication scored highest at 40, though "highest" is relative when the ceiling was 40 and the floor was 8. Both probes—**logical fallacies absent** and **reviewer panel verdict**—scored 40, but notably with evidence showing neither check was actually run. The logical_fallacies skill was never invoked, and no review_panel.md was generated.

This score reflects an absence of detected problems rather than a presence of verified quality. The run didn't produce obviously fallacious reasoning, but it also didn't subject itself to the adversarial scrutiny that would surface subtle issues. A score of 40 here essentially means "we didn't catch you making errors because we didn't look." This is the evaluation equivalent of passing a test you never took.

What this reveals about the run: the team may have prioritized moving forward over pausing to validate. Communication artifacts are often treated as polish to be added later, but without a review panel verdict or fallacy check, there's no evidence the core claims were stress-tested before being considered complete.

4.4.3 Weakest Dimension: Novelty Rigour (8)

At 8/100, Novelty Rigour represents the critical failure mode of this run. The two probes tell a damning story:

- **Augmented baseline catalog present** scored 10, with evidence showing "baseline_catalog has 0 rows." This means the run produced zero baseline comparisons. Without a catalog of known results, there is no way to determine whether any finding represents genuine novelty or rediscovery.
- **Strict-domination comparator run** scored 5, with "novelty_verdict.json not found." The comparator that would determine whether results strictly dominate known baselines was never executed.

The stage that produced this failure was clearly the **baseline establishment phase**. Before any novelty claims can be made, the run must populate a baseline catalog with prior art—known molecular energies, established operator counts, published gate complexities. This catalog wasn't just incomplete; it was empty.

Zero rows means zero comparisons were possible. The strict-domination comparator couldn't run because there was nothing to compare against.

This is a foundational failure. Everything downstream—claims of improvement, assertions of novelty, excitement about results—rests on sand. The run may have produced interesting outputs, but without baseline comparisons, "interesting" is indistinguishable from "already known" or even "worse than prior work."

4.4.4 Three Highest-Leverage Improvements

1. Populate the Baseline Catalog Before Starting Discovery The single highest-leverage fix is requiring a non-empty baseline catalog as a gate before the novelty search begins. This means compiling known results from literature, prior runs, or established benchmarks for the target molecules or problems. The baseline catalog should include at minimum: molecule identifiers, active space configurations, best-known energies with citations, and operator/gate counts from published methods. A run with 50 baseline rows would have transformed this evaluation.

2. Generate the Structured Pareto Archive The **pareto archive structured** probe scored 20 with evidence showing "archive rows: 0." A Pareto archive captures the trade-off frontier (e.g., accuracy vs. circuit depth) and preserves non-dominated solutions. Without this, there's no structured record of what the run explored. Implementing automatic Pareto archiving during the search loop—appending each non-dominated solution with its objective values—would improve Reproducibility and provide the raw material for novelty assessment.

3. Run the Strict-Domination Comparator and Generate novelty_verdict.json Even with a sparse baseline catalog, running the comparator produces a verdict file that honestly reports "no novelty proven" or "insufficient baselines." This file forces the run to confront its evidential status. The improvement here is procedural: make novelty_verdict.json generation a mandatory step before any run is considered complete. A verdict of "cannot assess" is more valuable than an absent verdict, because it surfaces the gap explicitly.

This run demonstrates what happens when execution outpaces verification infrastructure. The machinery to find novel solutions may have operated, but the machinery to prove they're novel was never built. A score of 23 is recoverable—but only if the next run treats baseline establishment and novelty verification as prerequisites, not afterthoughts.