📄 Peer Review Report

Title: *Quantum Computing for Chemistry Beyond Toy Molecules: Error Mitigation, Excited States, and Embedding Methods*
Author: Richard Murdoch Montgomery
Affiliation: Scottish Science Society, Edinburgh, Scotland
Recommendation: Minor revisions (see detailed comments below)

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1. Overall Evaluation

This manuscript offers a sophisticated, well-structured, and didactic review of the current state of quantum computing as applied to computational chemistry, focusing on the path from basic demonstrations to chemically meaningful simulations. The article balances formal theoretical exegesis, practical algorithmic insight, and implementation realism with clarity and breadth. It is both *pedagogically effective* and *technically substantive*, making it suitable for a wide readership interested in quantum algorithms, NISQ devices, and chemical simulation frontiers.

Nonetheless, a few refinements in presentation, precision, and contextual comparison would improve the paper's alignment with standards expected by a general-purpose or educational scientific journal.

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2. Strengths

- **Clarity and Rigor:** The manuscript is impressively written, using precise technical language and consistent mathematical formalisms. The notation is clean and consistent with conventions in the field.
- **Comprehensive Structure:** The article's modular breakdown—covering VQE foundations, error mitigation (ZNE, PEC, symmetry verification), excited state algorithms (VQD, SSVQE, qEOM), embedding methods (DFT embedding, DMET), and roadmap projections—is highly effective for both didactic and reference purposes.
- **Illustrative Figures:** Figures such as the VQE hybrid workflow (Figure 1), ZNE results (Figure 2), and error scaling benchmarks (Figure 5) enhance understanding and are clearly labelled.
- **Balanced Perspective:** The discussion section (Section 4) offers a refreshingly honest assessment of both capabilities and limitations, particularly around the scaling bottlenecks and the role of AI.
- **Original Code Appendix:** The Python code section is educational and aligns well with the tone and purpose of the article.

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3. Areas for Improvement

a. Title and Abstract

- *Title:* The phrase "Beyond Toy Molecules" is informal and might be perceived as dismissive. Consider revising to "Beyond Minimal Molecular Systems" or similar, which retains the intent but with more professional tone.
- *Abstract:* The final sentence suggests "some achieving chemical accuracy..." but does not specify which molecules or under what conditions. Either briefly name an example or moderate the claim.

b. Literature Integration

- The manuscript is rich in citations (especially in Section 7), but it could benefit from occasional in-text comparisons with recent competing methodologies:
  - For instance, some mention of *tensor networks* or *quantum-inspired algorithms* for chemistry (classical simulations using quantum concepts) would provide useful context.
  - Classical multi-reference methods (e.g. CASSCF, MRPT2) are mentioned but not explicitly compared with quantum ones—this would enhance Section 4.2.

c. Methodology and Results

- **Section 3:** Results are well-presented but could benefit from clearer **error bars or confidence intervals** where appropriate, especially in plots (e.g., Figure 3 and 5). While the qualitative narrative is solid, adding visual error bounds would strengthen credibility.
- **Figure 6 (Qubit Roadmap):** The right-hand side projection could mention assumptions underlying error rate evolution. Is this IBM's roadmap? If so, cite explicitly.

d. Technical Precision and Notation

- Equation (17): Notation could benefit from clarification—particularly what "ψ_virtual" exactly means and how it is included or approximated (MP2? DFT-based?).
- Equation (13) and (14): The constraint terms could be better explained for readers unfamiliar with the SWAP test.
- When introducing new acronyms (e.g. CPVQD, CIPEC), they should be defined the first time in both full and abbreviated forms.

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4. Minor Editorial Suggestions

- Throughout the manuscript, maintain British spelling consistently. In one or two places (e.g. "minimized" on p.20), American spelling creeps in.
- Check figure legends: Figure 2 refers to the "red star" and "purple diamond," but these colours may appear differently depending on print settings or greyscale. Consider adding shape descriptions or labelling directly in the image.
- The Python code is clear and instructive. For completeness, indicate which version of Qiskit or simulation backend was assumed.
- Consider breaking Section 4.5 ("Timeline Considerations") into bulleted milestones for even greater readability.
- The final paragraph of the conclusion is excellent, but the phrase "quantum interrogation" might raise eyebrows. Consider rephrasing: "quantum simulation" or "quantum analysis of nature's molecular systems."

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5. Suggested References to Add (Optional)

To enhance breadth, the following references could be considered:

- Elfving, V. E., et al. (2020). *How will quantum computers provide an industrial advantage in quantum chemistry?* arXiv:2009.12472
- Bravyi, S., et al. (2022). *Simulating Chemistry with Quantum Computers*. Nature Reviews Chemistry, 6, 1032–1048.
- Huggins, W. J., et al. (2021). *Unbiasing Fermionic Quantum Monte Carlo with a Quantum Computer*. Nature, 594(7862), 500–505.

✅ Final Recommendation

This manuscript is highly readable, authoritative, and pedagogically effective. It is well-suited for **average or upper-middle-tier interdisciplinary journals**, especially those catering to an audience transitioning from classical computational chemistry to quantum methods.

With minor revisions to formal tone, reference breadth, and visual/notation clarity, this article should be accepted and will likely serve as a valuable primer and roadmap in the field.