Here is a **peer review of the manuscript** titled *"Divide-and-Conquer Strong Correlation: How Embedding Transforms Exponential Walls into Engineering Problems"*, written in the style appropriate for an **average computational chemistry or quantum chemistry journal** (e.g., *Journal of Chemical Theory and Computation*, *Molecular Physics*, or *Chemical Physics Letters*).

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## Peer Review Report

**Title**: *Divide-and-Conquer Strong Correlation: How Embedding Transforms Exponential Walls into Engineering Problems*
**Author**: Richard Murdoch Montgomery
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**1. General Assessment**
This manuscript presents a comprehensive and well-structured overview of how modern quantum embedding techniques, particularly when combined with advanced solvers like DMRG and selected CI, have reframed the computational intractability of strong electron correlation in quantum chemistry into a series of tractable engineering decisions.

The exposition is rigorous yet accessible, merging theoretical clarity with practical insights and concluding with a detailed Python implementation (using PySCF and Block2). The article is of substantial pedagogical and methodological value for both early-stage researchers and established practitioners interested in multireference electronic structure methods.

The language, though dense, is coherent and suitably academic. The figures are informative, appropriately referenced, and effectively support the narrative. References are current and well-chosen.

**Recommendation**: Accept with minor revisions.

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**2. Strengths**

- **Clarity and Depth of Explanation**: The manuscript provides one of the clearest pedagogical introductions to the divide-and-conquer paradigm applied to strong correlation. Sections 2.2–2.4, covering DMRG, selected CI, and embedding theory, are especially well-written.
- **Use of Visual Aids**: The figures (especially Figures 1–4) are excellent in elucidating complex concepts such as exponential scaling, matrix product states, and DMET partitioning.
- **Relevance and Timeliness**: The discussion on the synergy between machine learning and quantum chemistry (Section 5.3), and the anticipation of quantum computing integration (Section 5.4), aligns with current and emerging trends.
- **Code Demonstration**: The inclusion of a detailed working Python example (Section 7) using accessible tools like PySCF is commendable and greatly enhances reproducibility and pedagogical value.

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**3. Points Requiring Minor Revision**

**3.1. Terminological Clarification**

- The manuscript uses “multireference” and “strong correlation” somewhat interchangeably. It would be beneficial to clarify early on (perhaps in the Introduction) that while they are related, they are not synonymous. Some systems may require a multireference treatment without strong correlation, and vice versa.

**3.2. Benchmark Discussion (Section 4)**

- While systems such as $Cr_2$ and FeNO are appropriately chosen as challenging benchmarks, the justification for these specific examples could be slightly expanded. For example, why was the FeNO complex preferred over classical ferrocene-type systems?
- The bar chart in Figure 6 is useful, but lacks information about the basis sets used, computational details (e.g., which NEVPT2 variant), and what “reference values” are being used. A short methodological note accompanying the figure would improve transparency.

**3.3. Scope of Limitations (Section 5.2)**

- The manuscript briefly mentions challenges in treating extended delocalised correlation and inter-fragment coupling. However, more critical discussion would strengthen this section. For instance, methods like Self-Energy Embedding Theory (SEET) or Localized Active Space Self-Consistent Field (LASSCF) could be briefly referenced as complementary approaches addressing these issues.

**3.4. Code Comments and Portability**

- While the code provided is thorough, a short note indicating the version compatibility (e.g., PySCF 2.1+, Python 3.10) and hardware requirements (e.g., RAM, cores) would be helpful for average users.

**3.5. References**

- The bibliography is excellent and comprehensive. However, a few key review articles could be added, especially those covering the integration of ML and quantum chemistry (e.g., von Lilienfeld et al., 2020, *Nature Reviews Chemistry*).

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**4. Suggestions for Enhancement (Optional)**

- **Extended Examples**: If space allows, a second case study using a biologically relevant metal center (e.g., Zn in metalloenzymes or Cu in hemocyanins) could showcase the flexibility of the method beyond iron-based systems.
- **Machine Learning Integration**: While future prospects are mentioned, a brief mock-up or hypothetical application (e.g., predicting fragment partitions using a GNN) would illustrate how the field could move toward automation.
- **User-facing Tools**: Mention of GUI-based or notebook-integrated workflows (e.g., PySCF with JupyterLab) might help engage a broader computational audience.

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**5. Conclusion**
This is a well-crafted and forward-thinking article that would make a valuable contribution to a standard periodical in quantum chemistry or computational materials science. Its conceptual clarity, balance between theory and application, and inclusion of real code distinguish it as an excellent teaching and reference piece.

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## Reviewer Recommendation:

☑ **Accept with Minor Revisions**