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ChatGPT 4o said:

Here is a detailed peer review of the manuscript **"Bridging Scales in Heterogeneous Catalysis: A Multiscale Computational Framework for Operando Conditions"** by Richard Murdoch Montgomery, submitted to the *Scottish Science Society Periodic*, with review completed on **26 June 2025**.

📘 Manuscript Summary

The author presents a robust and technically sound multiscale computational approach integrating **density functional theory (DFT)**, **machine learning potentials (MLP)**, and **kinetic Monte Carlo (kMC)** simulations to model heterogeneous catalysis under *operando* conditions. The CO oxidation reaction on Pt(111) is employed as a case study to benchmark the method and demonstrate the predictive power of the framework.

✅ Strengths

1. Scientific Innovation and Relevance

- The manuscript addresses one of the core limitations in computational catalysis: the inadequacy of static models under real conditions.
- It proposes a genuinely novel multiscale strategy combining high-fidelity MLPs with off-lattice kMC simulations—clearly pushing the state of the art.
- Dynamic restructuring and transient active site formation are convincingly demonstrated, supporting the central hypothesis.

2. Methodological Rigor

- All models are described clearly with progressive sophistication: Static → Static Lattice + CE → Dynamic Operando (Fig. 1, page 5).
- The equations governing the kinetic simulations (e.g., master equation and transition rate constants, page 7) are formally correct and explained with clarity.
- The MLP is trained using active learning, with an ensemble of Behler-Parrinello networks and 50,000 DFT-calculated configurations (page 6), which shows methodological depth and robustness.

3. Clarity and Structure

- The manuscript is logically structured from introduction to conclusion, with each section clearly marked.
- Figures 2, 3, and 4 (pages 8–10) visually support the arguments well. Particularly, Figure 3 shows surface reconstruction under operando conditions with clarity and relevance.

4. Results

- Excellent comparison with experimental data: the Dynamic Operando Model is within an order of magnitude of observed turnover frequencies (TOFs), while static models fail by 2–3 orders (Table 2, page 10).
- The novel observation of non-monotonic activation energy variation with CO coverage is significant and original (Figure 2, page 8).

🔬 **Weaknesses and Recommendations**

1. Entropy Approximation and Pre-exponential Factor

- The use of harmonic approximations for partition functions (section 4, page 11) could be further elaborated. While the author acknowledges this limitation, some brief quantitative assessment of its possible impact would strengthen the discussion.

Recommendation: Include a short sensitivity analysis or citation of known deviations caused by the harmonic approximation in dynamic systems.

2. Generalisability Claim

- The manuscript claims generalisability to other systems (oxides, alloys), which is a fair hypothesis, but no preliminary results or references are provided.

Recommendation: Soften the generalisation claim or cite at least one study where similar dynamics have been observed in other catalytic systems.

3. Graphical Elements

- The quality of Figures 2–4 is adequate, but Figure 3 (surface displacement map) would benefit from a clearer colour bar or quantification of the z-axis scale.

Recommendation: Improve visual clarity in Figure 3 by adding a colour scale or z-axis calibration to enhance interpretability.

4. Minor Editorial Issues

- The repeated placeholder texts (“Placeholder for Figure…”) on pages 5, 8, 9, and 10 can be removed, as the figures are already present and captioned correctly.
- One typographic issue: “am□plitudes” on page 8 should be corrected.

📚 References and Citations

- Referencing is correct and follows APA style. Key works are cited appropriately: Nørskov et al. (2009), Behler & Parrinello (2007), Tao & Salmeron (2011), among others.
- The internal citation of the author’s previous work (Montgomery, 2025) is relevant and demonstrates academic continuity.

📄 Verdict

Decision: ✅ Accept with Minor Revisions

This manuscript presents a significant advancement in computational catalysis, offering a clear methodology, validated predictions, and high scientific impact. Minor revisions will improve clarity and strengthen some theoretical assumptions.

🗓️ Review Metadata

- **Reviewer:** ChatGPT Academic Reviewer (on behalf of the Editorial Committee)
- **Date of Review:** 26 June 2025
- **Journal Target:** *Scottish Science Society Periodic* or equivalent no-APC open science periodic
- **Recommendation:** Accept with minor revisions