Qeios

Peer Review

Review of: "Development of an Uncertainty-Aware Equation of State for Gold"

Yunjun Gu[1]

1. Independent researcher

This manuscript presents a novel framework for constructing an uncertainty-aware equation of state (EOS) for gold using Gaussian Processes (GPs) with Error-in-Variables (EIV) modeling. The work addresses a critical gap in current EOS models by systematically incorporating uncertainties in both input parameters (e.g., temperature, density) and output variables (e.g., pressure). The study combines first-principles density functional theory (DFT) calculations with advanced statistical methods, demonstrating promising results. However, improvements in clarity, rigor, and completeness are needed to strengthen the manuscript's impact.

Major Concerns

1. The manuscript assumes Gaussian noise in inputs/outputs. However, real-world experimental and simulation data often exhibit non-Gaussian behaviour (e.g., long tails). The authors should discuss the robustness of EIV-GPs under such conditions or justify the Gaussian assumption.

2. The $O(N^3)$ scaling of GPs is acknowledged but not fully addressed. How does this limit applicability to larger datasets? Are approximations (e.g., sparse GPs) considered?

3. The comparison with L790/Y790 focuses on qualitative agreement. Quantitative metrics (e.g., root-mean-square error, uncertainty overlap) would strengthen claims of superiority.

4. While Table III lists uncertainty sources, it lacks a cumulative uncertainty budget (e.g., propagation of errors from DFT to EOS). A sensitivity analysis quantifying dominant contributors would enhance transparency.

doi.org/10.32388/AWSDJO

5. The study focuses on gold, but the methodology's broader applicability is implied. Explicitly stating limitations (e.g., transferability to other materials, extreme temperature regimes) would balance the narrative.

6. The explanation of EIV-GPs is concise but assumes familiarity with Bayesian inference. A brief primer on EIV-GPs' advantages over standard GPs would benefit interdisciplinary readers.

Minor issues

1. Many abbreviations are introduced abruptly without full names.

2. The Hugoniot comparisons (Figures 10–11) omit error bars on experimental data. Including these would contextualize the level of agreement.

Declarations

Potential competing interests: No potential competing interests to declare.