

Bayesian Calibration with Optimized Surrogate Models for Materials and Engineering

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Abstract

Predictive modeling plays a central role in modern materials design, enabling the exploration of structure–property relationships and the acceleration of materials discovery. However, the reliability of such models critically depends on the accurate calibration of model parameters using experimental data that are often sparse, noisy, and expensive to obtain. Conventional calibration approaches typically rely on deterministic error minimization between simulations and experiments, providing point estimates that ignore measurement uncertainty, model inadequacy, and variability across processing conditions. In materials applications - where experiments may be costly, destructive, or time-consuming - these limitations can severely compromise model credibility and downstream decision-making.

Bayesian calibration offers a natural framework for materials modeling by explicitly accounting for experimental uncertainty, model discrepancy, and prior knowledge derived from physics-based constraints, literature data, or previous characterization campaigns. By treating calibration as a probabilistic inference problem, Bayesian methods yield posterior distributions over material and model parameters, enabling uncertainty-aware predictions of material behavior rather than single best-fit responses. This capability is essential for quantifying confidence in property predictions, guiding additional experiments, and supporting risk-informed materials design.

To make Bayesian calibration tractable for computationally intensive materials models, we employ a surrogate-assisted approach based on Gaussian process emulators. These surrogates enable efficient exploration of parameter spaces while preserving uncertainty propagation from model inputs to material responses. A central contribution of this work is the automatic optimization of surrogate kernels, improving emulator fidelity under the small-data regimes typical of materials characterization.

The proposed approach is connected to our open-source Python package ACBICI for Bayesian calibration. We demonstrate the methodology

through materials and engineering case studies, illustrating how optimized surrogate models enable robust Bayesian calibration and deliver actionable uncertainty quantification for these case studies.

References

- [1] C. Schenk, I. Romero (2026): <https://gitlab.com/schenkch/ACBICI.git>.
- [2] C. Schenk, I. Romero (2026): A Framework for the Bayesian Calibration of Complex and Data-Scarce Models in Applied Sciences, arXiv, <https://arxiv.org/abs/2601.22890>.