

KadiAlgent: Active learning–driven interoperable workflows for multi-objective materials optimization

Author:

Giovanna Tosato

Co-authors:

Leon Merker, Monika Vogler, Ian Mendonca, Michael Selzer, Arnd Koeppe

Material design frequently requires navigating high-dimensional parameter spaces to identify configurations that balance competing objectives, demanding smarter strategies.

We present a methodological contribution: KadiAlgent, an active-learning framework that enables interoperability between the Kadi ecosystem and external execution infrastructures, including the FINALES system for experimental workflows and HPC clusters for large-scale simulations.

The resulting predictive and scalable pipelines are applicable across both computational and experimental domains, thereby enabling transferable materials discovery workflows.

KadiAlgent performs single- and multi-objective Bayesian optimization, quantifying knowledge and uncertainty through probabilistic surrogate models. This uncertainty-aware approach identifies promising regions of complex design spaces and thereby the most informative parameter configurations with relatively few evaluations compared to classical methods. The result is efficient, data-driven materials design that maximizes the information gained from each iteration, reducing the need for resource-intensive simulations or experiments. By employing highly customizable, multiphase generation strategies, KadiAlgent supports automated exploration and optimization across different domains.

The flexibility and effectiveness of this framework are demonstrated in two energy-storage use cases spanning both experimental and simulation-driven workflows. In the first [1], multi-objective optimization of Sodium-ion battery formation protocols is performed through a human-in-the-loop workflow that orchestrates experiment planning and execution. By establishing interoperability between Kadi4Mat and the FINALES framework, the combined system coordinates automated assembly, cycling, and data upload across the POLiS Materials Acceleration Platform, targeting the end-of-life performance and efficient formation of sodium-ion coin cells as competing objectives. In the second use case [2], we model the aging of Ni-GDC anodes in solid-oxide fuel cells and identify optimal simulation parameters from experimental microstructure data. HPC-executed multiphase-field simulations with the suggested parameter configuration are automatically triggered at each iteration as part of a fully

automated simulation campaign, demonstrating the framework's transferability to computationally intensive parameter spaces.

[1] G. Tosato, L. Merker, M. Vogler, M. Selzer, and A. Koeppel. Accelerating battery research with an ai interface between FINALES and Kadi4Mat. arXiv preprint arXiv:2605.00909, 2026.

[2] R.K. Jeela, G. Tosato, M. Ahmad, M. Wieler, A. Koeppel, B. Nestler, and D. Schneider. Enhancing solid oxide fuel cells development through Bayesian active learning. Advanced Energy Materials, page 2501216, 2025.