Autonomous Optimization of Perovskite Solar Cell Thin Films via Robotic Spin-Coating and Bayesian Optimization

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1. Introduction

The development of high-efficiency perovskite solar cells relies heavily on identifying the precise combination of processing conditions and material compositions. Poor reproducibility and sensitivity to processing parameters have made it difficult to systematically optimize perovskite thin films across labs. The high dimensionality of the processing parameter space makes traditional trial-and-error methods poorly equipped to navigate the experimental search space. Automated, self-driving laboratories offer a solution by coupling robotic synthesis with machine learning algorithms.

In this work, we present a fully automated, closed-loop spin-coating platform driven by a high-dimensional Bayesian optimization framework to autonomously optimize the synthesis of perovskite thin films.

2. Platform and Software Orchestration

To enable autonomous optmization, we employ the SpinBot platform with custom modifications for Bayesian optimization closed loop integration. The system autonomously performs spin coating, thermal annealing, high-quality optical imaging, and spatially resolved photoluminescence (PL) and absorption mapping.

We developed a custom software orchestration framework that successfully bridges the robotic synthesis hardware with a Bayesian Optimization loop, enabling continuous, unassisted experimental iterations.

3. High-Dimensional Optimization

The optimization of perovskite film quality is framed as a multi-objective problem, maximizing both overall PL intensity and spatial film uniformity. The processing parameter space consists of 10 to 20 continuous and categorical variables, including precursor and antisolvent dispense timing, multi-stage spin speeds and durations, as well as annealing temperatures and times.

To attempt to navigate this high-dimensional space, we utilize the Ax platform [1] for Bayesian optimization. Alongside standard BO surrogate models, we implement BONSAI [2], which is specifically designed to handle high parameter dimensions by disregarding irrelevant parameters from the optimization.

4. Preliminary Results and Future Work

Initial optimization runs have demonstrated the platform's ability to autonomously explore the parameter space and identify processing conditions that yield improved PL intensity and film uniformity. Future work will focus on further refining the optimization algorithms, incorporating additional characterization techniques, and ultimately applying the optimized processing conditions to fabricate high-efficiency perovskite solar cells.

References

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