Autonomous OPV Device Optimization

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Motivation

▸ **Complexity of OPV Optimization:**
Organic Photovoltaics (OPV) offer promising applications, but optimizing them is challenging and time-consuming

▸ **Complex Parameter Interactions:**
Conventional methods can be inefficient in handling the correlations and interactions among OPV parameters.

▸ **Need for Acceleration:**
Historically, it takes decades to transfer new technologies from the lab to industrial applications.

Approach

▸ **Autonomous Optimization:**
We introduce an AI-guided closed-loop approach for OPV devices.

▸ **Automated Fabrication and Characterization**
LineOne, our automated materials and device acceleration platform is able to fabricate and characterize fully functional OPV devices

▸ **Early Prediction Model:**
We employ a Gaussian Progress Regression (GPR) based early prediction model of the efficiency, using cheap proxy absorption measurements and an optical model.

▸ **Demonstration:**
We demonstrate the approach be optimizing a ternary OPV system (PM6:Y12:PC70BM) in a four-dimensional parameter space
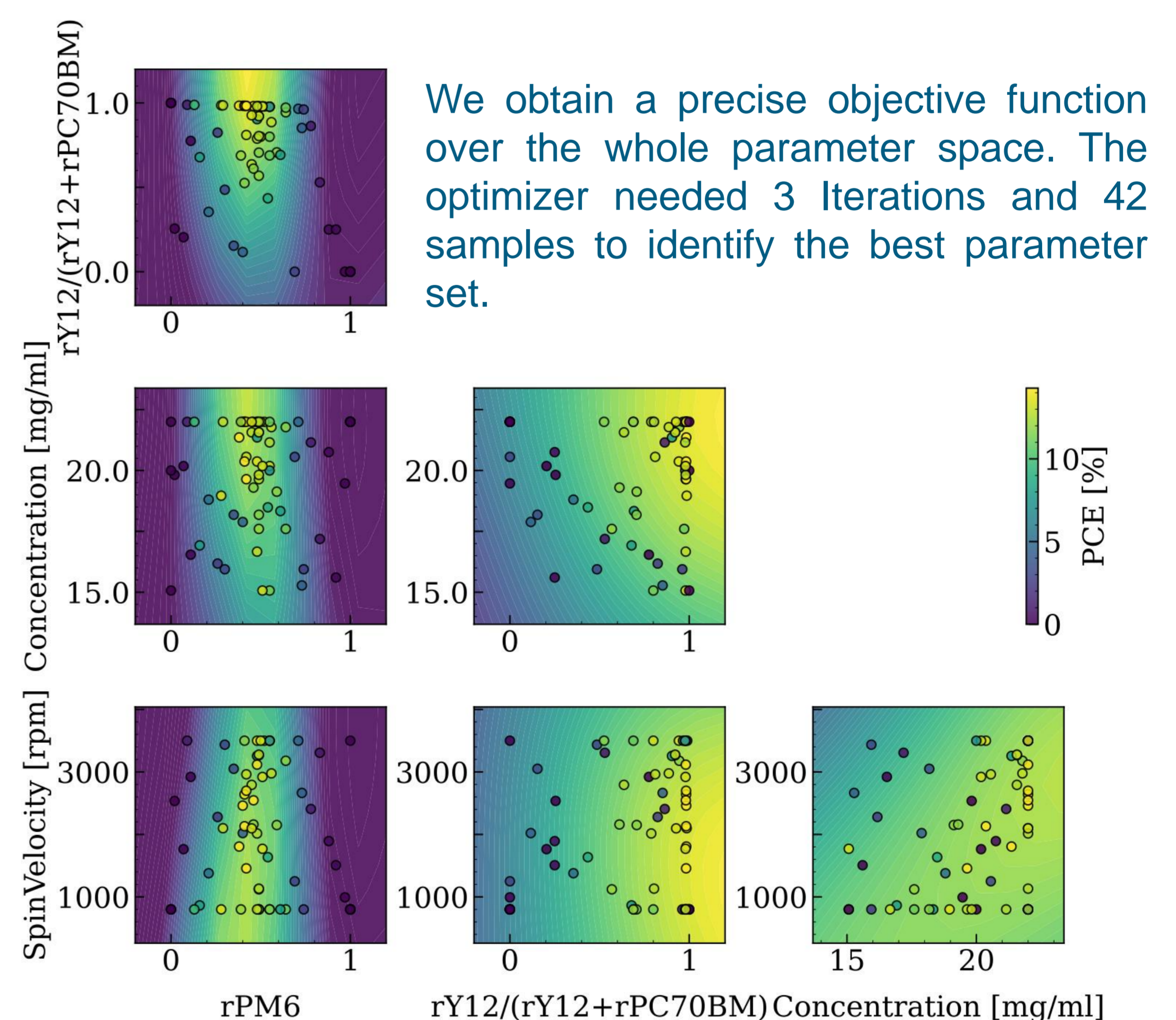
Closed-Loop Optimization
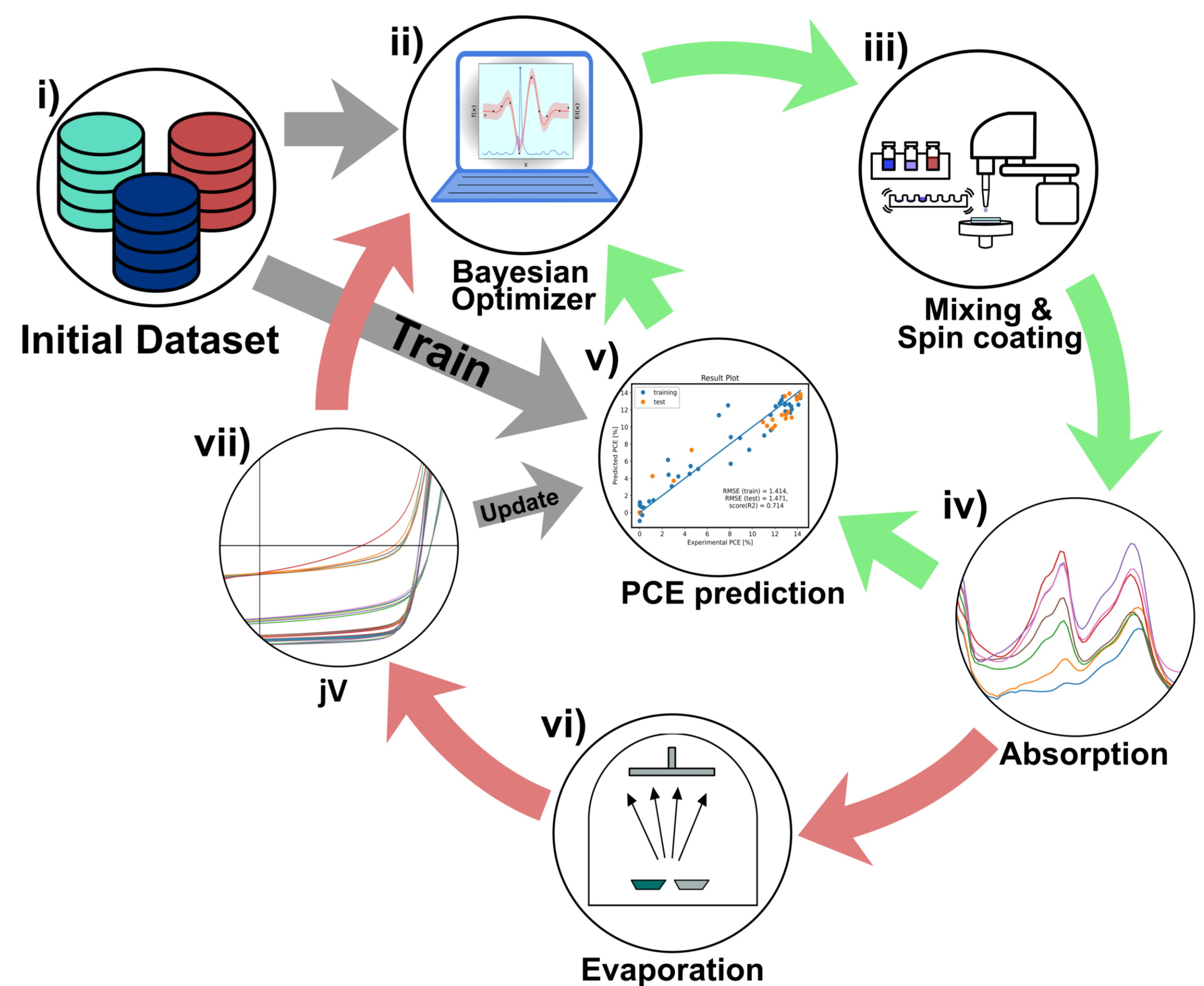
Early Prediction Model
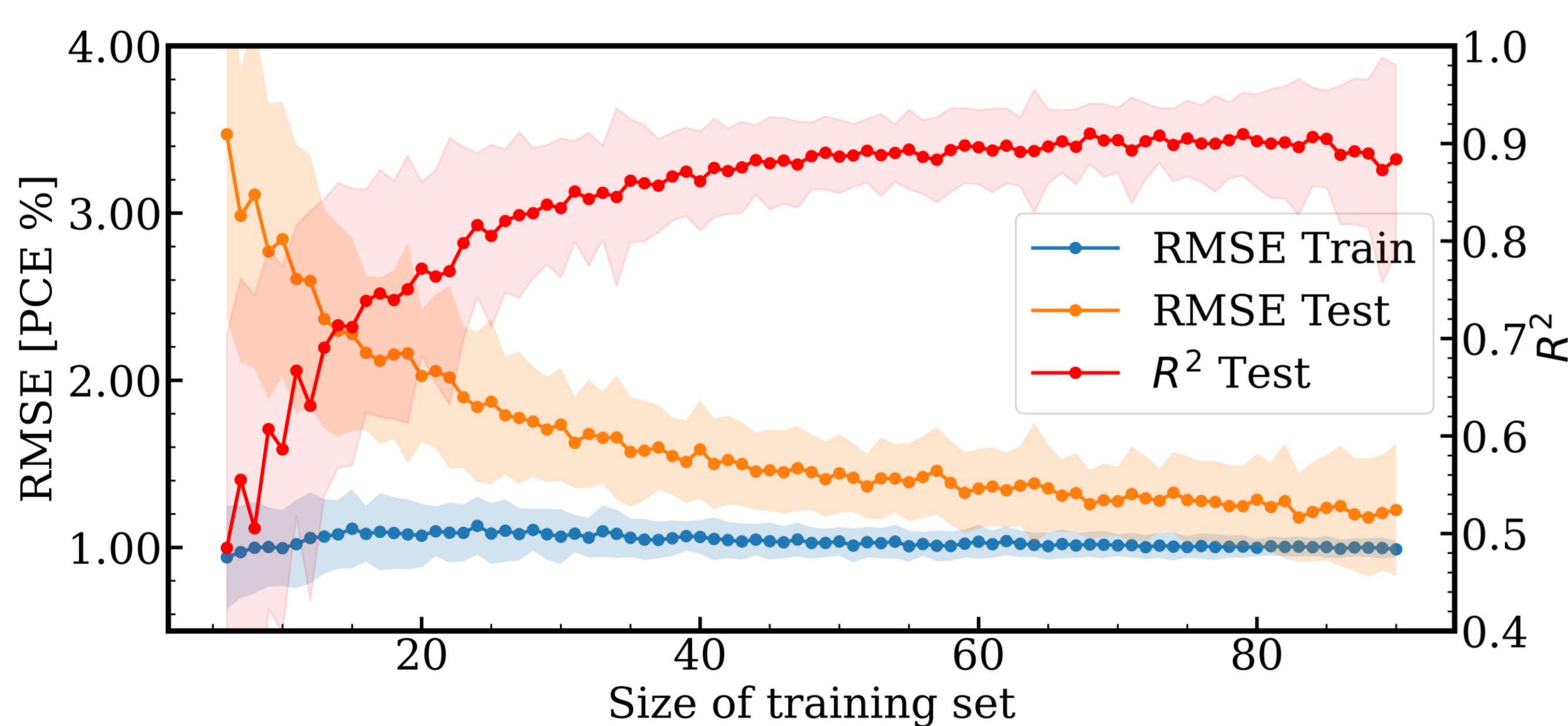
Features obtained by fitting the absorption spectrum of the active layer with an spectral model are used to predict the PCE of the devices.

Results

We obtain a precise objective function over the whole parameter space. The optimizer needed 3 Iterations and 42 samples to identify the best parameter set.

Conclusion and Outlook

▸ **Efficient Autonomous Optimization:** Our self-driving lab, guided by Bayesian Optimization, streamlines complex optoelectronic device optimization, conserving resources and accelerating technology advancement.

▸ **Efficient Material Development:** Understanding the influence and importance of composition and process parameters is important for developing new materials, and efficient device optimization.

▸ **Data Collaboration**: Adhering to FAIR principles, we encourage data reuse and collaboration, potentially enhance models and accelerate material discovery.

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