Advanced Characterization and Degradation Analysis of Perovskite Solar Cells using Machine Learning and Bayesian Optimization

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Context & Scale

- Poor stability is a major barrier to the commercialization of perovskite solar cells.
- With so many factors to consider, it often takes years to understand performance bottlenecks and optimize the design process.
- We combine physics modeling, machine learning, and experimentation to better understand the complex relationship between device performance and underlying properties.

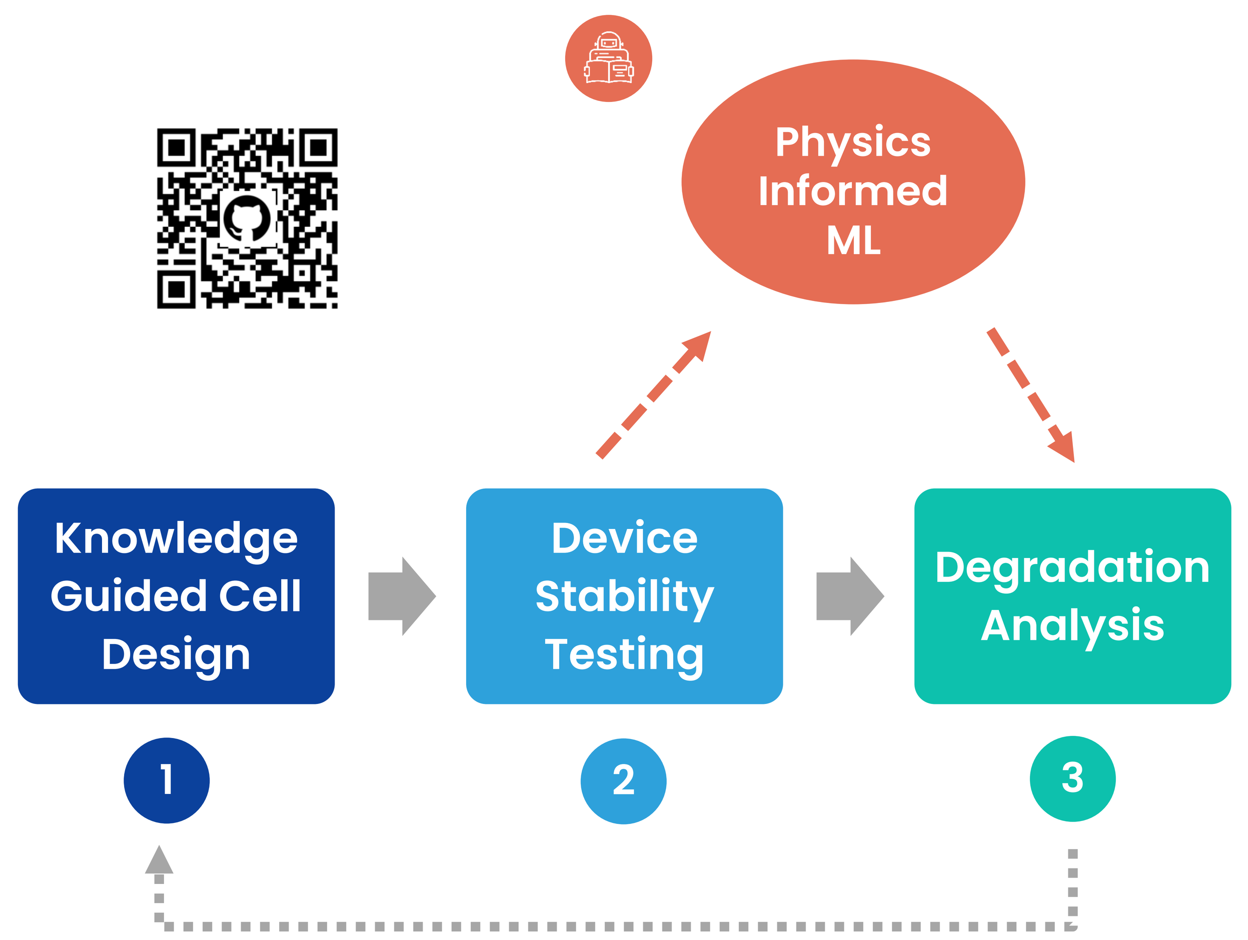
→ Gain insights into performance and degradation

→ Reduce the need for time-consuming and laborious characterization techniques

→ Flexible & scalable approach

Methodology

We develop a machine-learning-assisted characterization pipeline that leverages the information hidden in commonly-available testing data to accelerate the design process.



References

1. M. Koopmans, V. M. L. Corre and L. J. A. Koster, *Journal of Open Source Software*, 2022, 7, 3727.
2. A. Julien, J.-B. Puel and J.-F. Guillemoles, *Energy Environ. Sci.*, 2023, 16, 190–200.
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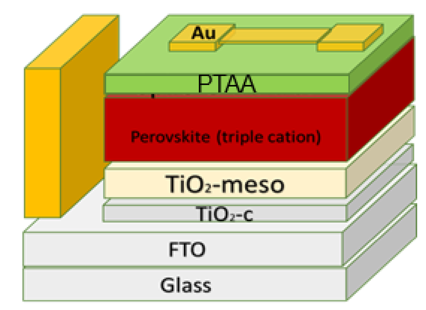
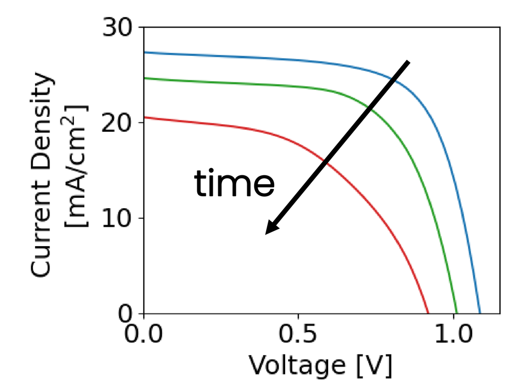
Results

1. We consider in-house triple-cation perovskite solar cells with different concentrations of PbSCN and define the parameters of a 1D drift-diffusion model [1] based on prior experience and the literature [2].

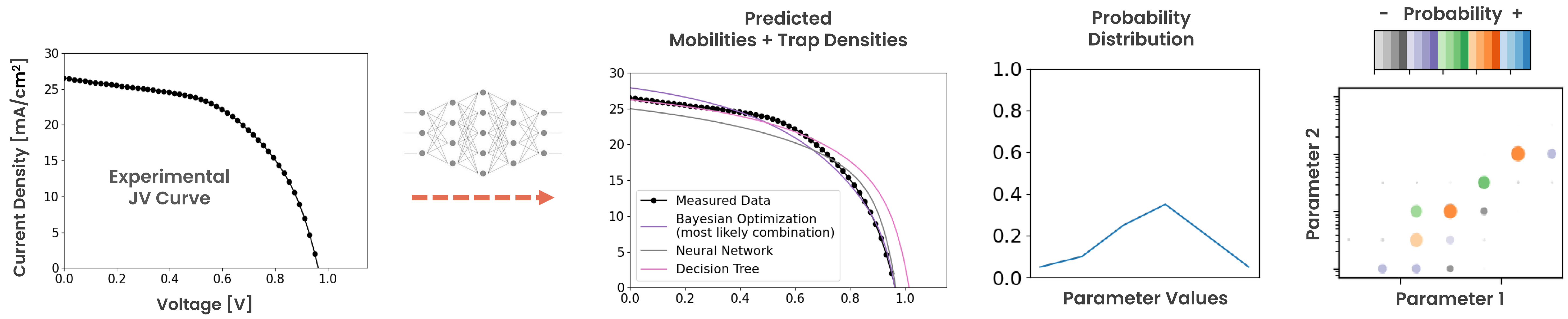




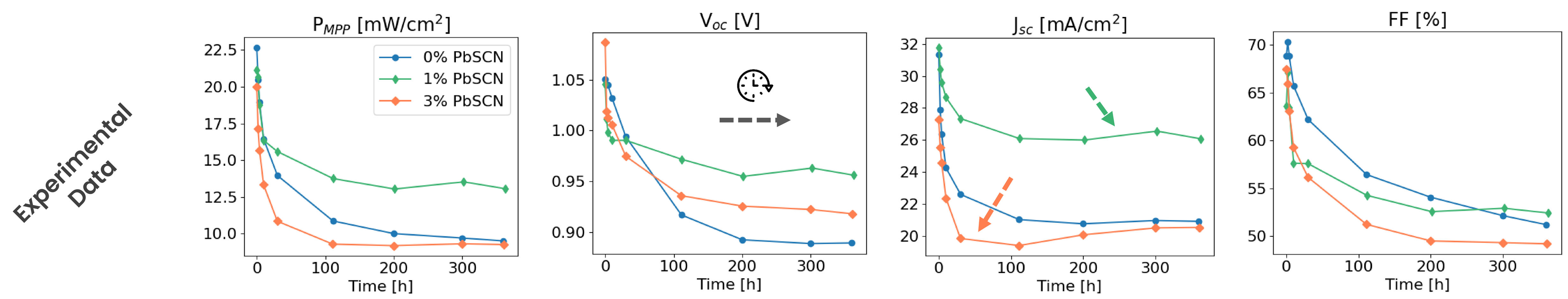
2. We age the cells following the ISOS-L1 protocol.
→ irradiance of 1.45 Suns & ambient temperature of 25°C

We train classical machine learning algorithms like neural networks [3] and decision trees on simulated current-voltage (JV) curves and test their ability to predict material and interface properties from experimental data.

Using Bayesian optimization, we can also find a set of possible solutions, build probability distributions over each parameter, and quantify prediction uncertainty.



3. We repeat this process to monitor the evolution of the JV properties and cell parameters over time.



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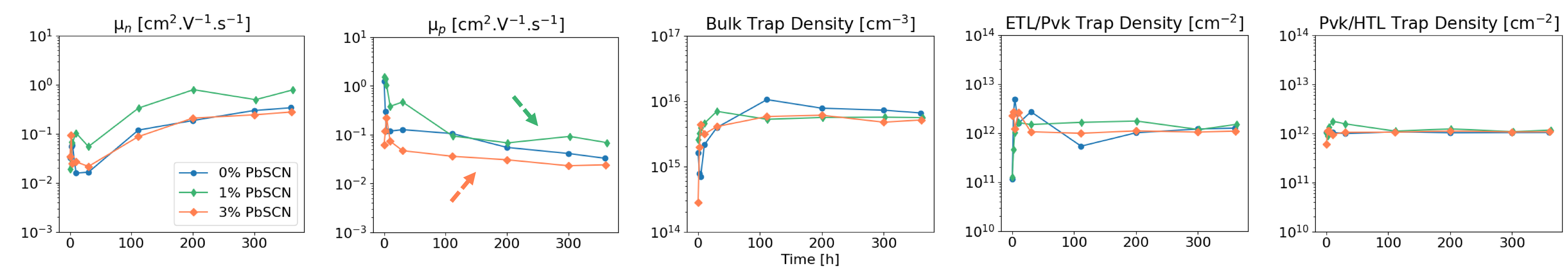
Supplemental ML Predictions
(Expected Values from Bayesian Optimization)



Perspectives

- Balance exploration and exploitation of the Bayesian optimization search space using acquisition functions.
- Evaluate additional neural network architectures/machine learning algorithms and optimize their hyperparameters.
- Consider complementary device measurements to increase parameter prediction capability and certainty.