



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

Joseph Chakar, Arthur Julien, Karim Medjoubi, Jorge Posada, Jean-François Guillemoles, Jean Baptiste Puel, Yvan Bonnassieux

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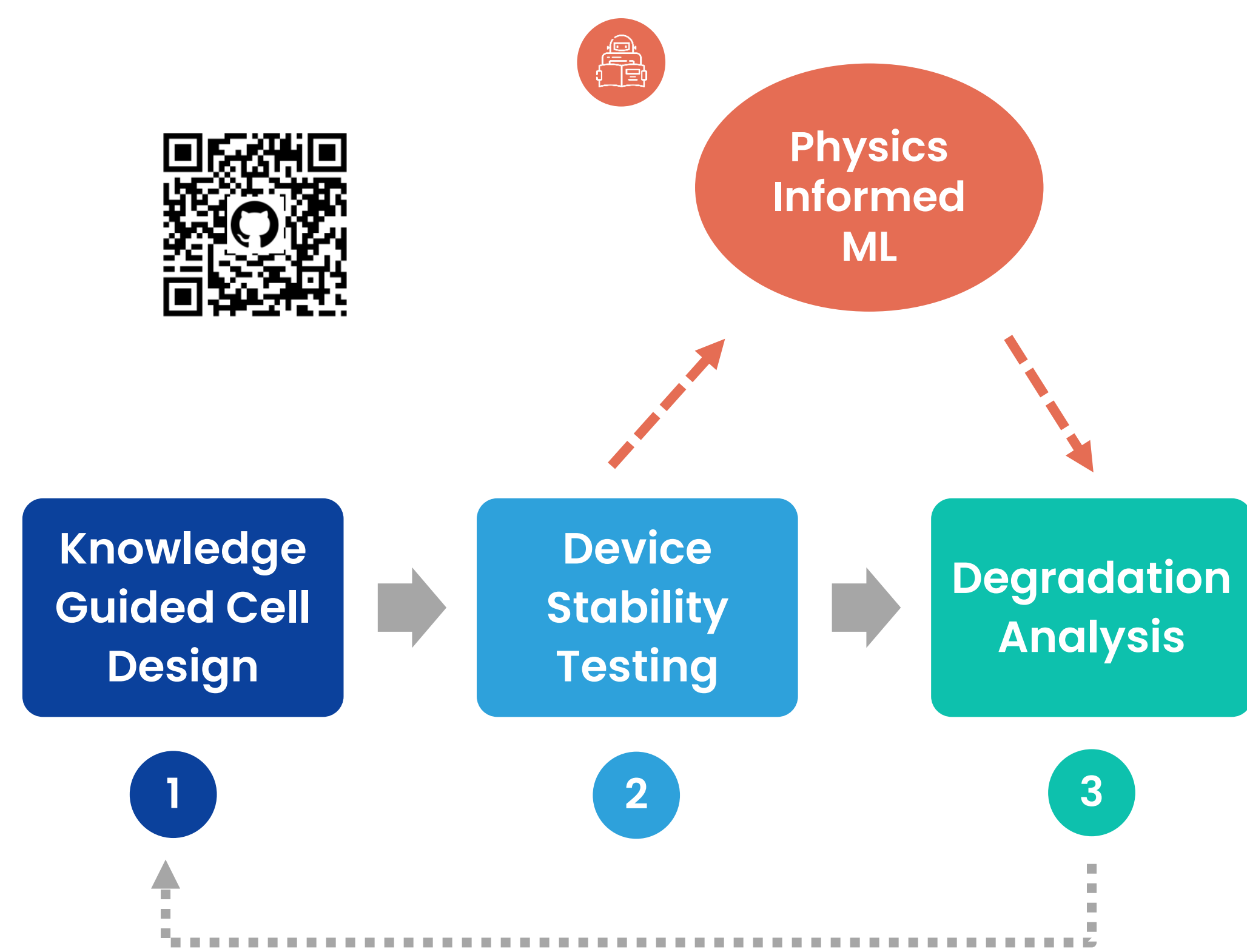
Joseph Chakar (joseph.chakar@polytechnique.edu), Arthur Julien, Karim Medjoubi, Jorge Posada, Jean-François Guillemoles, Jean-Baptiste Puel, and Yvan Bonnassieux

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.

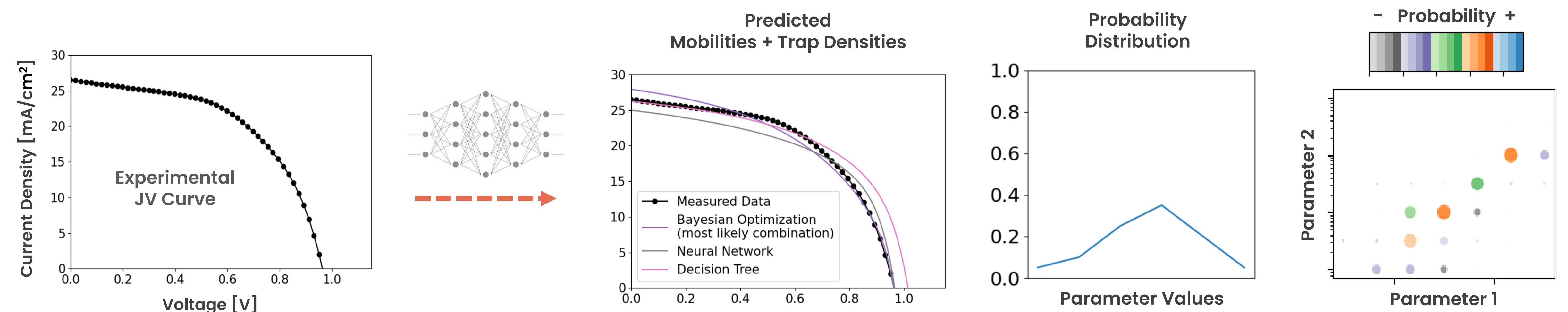


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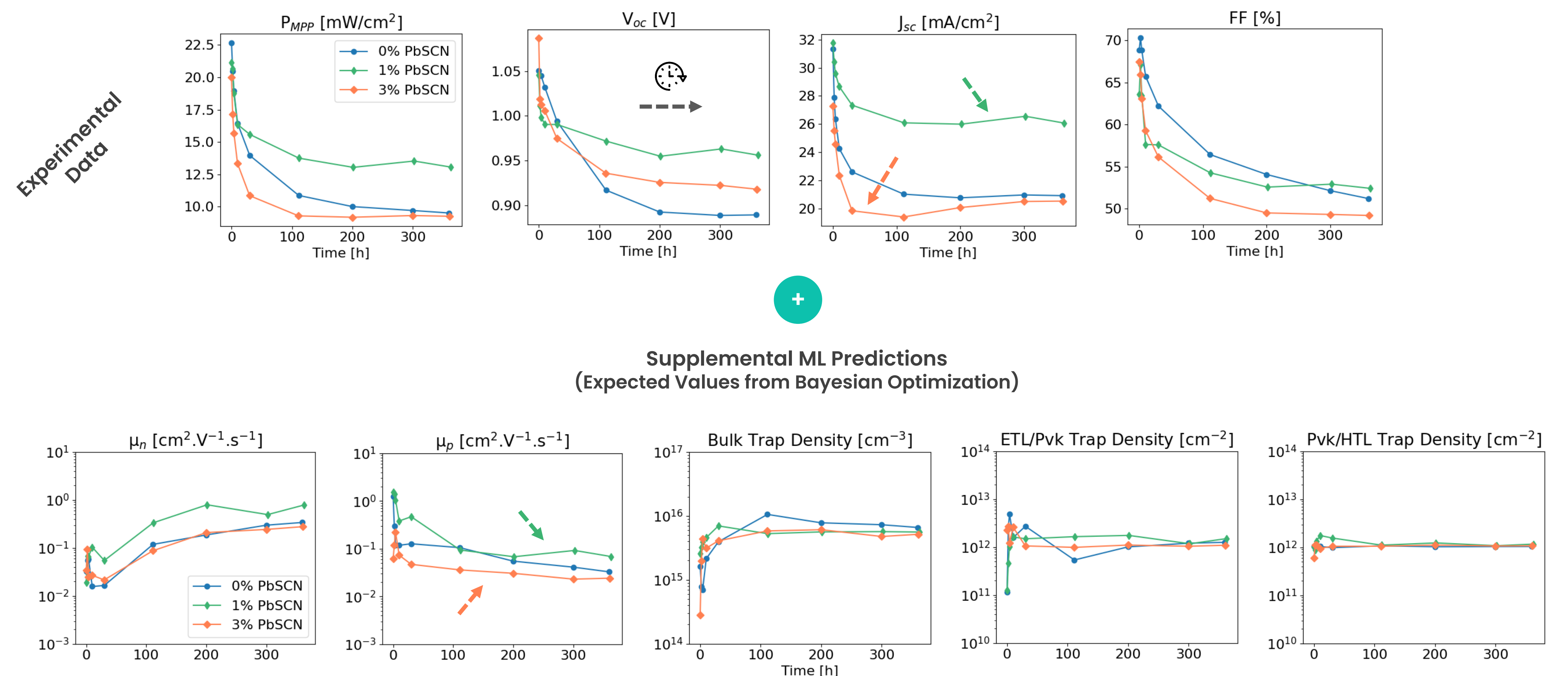
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Results

- 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].
 - 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.



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



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.