

Optimizing Perovskite Solar Cell Film with ViperLab

Sector

Renewable Energy & Materials Science

Impact

Accelerated Materials Optimization

Overview

Perovskite solar cells (PSC) are at the forefront of renewable energy technology due to their high efficiency and low production cost. A critical step in their manufacturing pipeline is optimizing the perovskite active layer, which determines the device's ability to convert sunlight into electricity. Atinary's machine learning (ML) optimizer, Falcon, was used to tune the active layer's composition and processing conditions to achieve a high-quality crystal structure with optimal optical and electronic properties.

Challenge

- **Experimental burden:** Manual parameter exploration is time-consuming and resource-intensive.
- **Large search space:** The perovskite film synthesis is composed of various constrained parameters such as the layer composition, and spin coating parameters such as the spin speed and duration.
- **Unclear performance objectives:** Typically, the film is the first step in a multistep manufacturing process whose performance is typically only evaluated at the end once the final cell is produced. It is a challenge to find good intermediate objectives that can already quantify the film electronic properties from its photoluminescence spectrum.

Use-case

Using Atinary's no-code AI platform, SDLabs, ViperLab automated the search for optimal perovskite layer properties. Atinary's optimizer explored a five-dimensional parameter space, which included the parameters for material composition, spin-coating speed, and annealing time. Through iterative optimization:

1. Stock solutions of cations were mixed based on Falcon's suggestions via a robotic platform. These stock solutions were spin coated on a support to create the film.
2. Two key metrics were considered to evaluate the photoluminescence spectra: full width at half maximum (FWHM) and the Photoluminescence Quantum Yield (PLQY). A narrower width suggests a more ordered crystal structure, essential for efficient charge transport, and a high PLQY indicates better photon-to-electron conversion efficiency.

With a batch size of 16, the PSC team at ViperLab could track the progression of their optimization efforts, using the data analytics module on Atinary's SDLabs platform. The most promising optimality region was quickly identified — after 80 samples within just 5 iterations.





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Benefits

- **Efficiency:** Reduced experimentation time with fewer iterations.
- **Enhanced performance:** Optimized films demonstrated superior photonic properties.
- **Scalability:** The method is adaptable for other thin-film materials.
- **Actionable insights:** Advanced understanding of parameter-property relationships in perovskite layers.

Resources

- [Link](#) to **Atinary - ViperLab project information**
- More about [ViperLab](#)

