

From Trial-and-Error to Learn-by-Experiment: The Future of Materials Research in Perovskite and Organic Photovoltaics

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Abstract: The next major change in perovskite and organic photovoltaic research may not come from a new material or device architecture, but from a new way of doing and analyzing experiments. Conventional trial-and-error optimization, often a one-variable-at-a-time (OVAT) approach, typically varies a limited number of parameters sequentially, making it difficult to resolve interactions within the increasingly complex processing spaces of complex, multilayer solar cells and demands a large number of experiments. We argue that robotic experimentation combined with machine learning can fundamentally alter this approach. The key advantage of robotics is not simply higher throughput, but highly precise and reproducible fabrication together with comprehensive recording of processing and environmental conditions. This transforms individual experiments into reliable, machine-readable data points and provides the foundation for machine learning to explore multidimensional parameter spaces, identify hidden correlations and autonomously select informative experiments. Optimization can consequently move beyond maximizing power-conversion efficiency toward understanding how parameters interact, with simultaneous consideration of efficiency, lifetime, stability, reproducibility, resource consumption and environmental impact. Such a transition could replace sequential trial-and-error optimization with reproducible, data-rich and closed-loop experimentation. Rather than replacing researchers, robotic laboratories may enable them to investigate materials and processing spaces that are too complex to explore manually. We propose that the long-term impact of autonomous experimentation in photovoltaics will therefore be measured by how much more can be learned from every experiment.

Keywords: autonomous experimentation; machine learning; organic and perovskite solar cells

1. Introduction

Perovskite and organic photovoltaics have developed at remarkable speed, largely through a trial-and-error paradigm: researchers vary a limited number of processing conditions sequentially, guided as much by experience as by systematic understanding and results are often difficult to reproduce even under nominally identical conditions. This becomes a real limitation as the number of interacting variables, such as material composition, solvent system, deposition conditions, quenching, annealing, device architecture grows. This is especially true for solution-processing steps such as antisolvent and gas quenching, whose film-formation mechanisms are still being systematically mapped [1].



One response has been Materials Acceleration Platforms (MAPs): robotic, automated platforms that prepare and characterize many material and process combinations under controlled conditions, described by Wagner et al. as a framework for distributed, automated materials development [2].

Du et al. demonstrated a robot-based platform fabricating and characterizing over 100 processing variations in 70 h, producing a dataset structured enough for machine-learning-based prediction [3].

In perovskites, Zhao et al. used high-throughput robotic learning to discover a temperature-induced stability reversal, revealing relationships conventional workflows would likely have missed [4].

Combining automation with machine learning is the next step: Zhang et al. demonstrated a machine-learning-guided robotic platform for optimizing perovskite thin-film parameter spaces, moving beyond conventional parameter-by-parameter tuning [5]. A similar high-throughput, machine-learning-guided approach has been used to fabricate and optimize quasi-2D Ruddlesden–Popper perovskite solar cells [6]. This has evolved toward self-driving laboratories, where Zhang, Hauch and Brabec proposed the Autonomous Materials and Device Acceleration Platform (AMADAP), combining robotic synthesis, fabrication, characterization, and AI-driven decision-making [7], into a self-driven experimental workflow [8].

A 2025 review outlined the emerging self-driven AMADAP laboratory concept [9], and Gao et al. recently coupled ML-driven molecular discovery directly to robotic device fabrication [10], reaching 27.22% efficiency while substantially improving reproducibility. Cakan et al. similarly reported a fully self-driving experimental workflow for perovskite photovoltaics, closing the loop between robotic synthesis, characterization, and machine-learning-guided decision-making [11]. The same shift is emerging in organic photovoltaics, where AI- and machine-learning-integrated pipelines are increasingly used to guide molecular and process design [12].

Robotics' deeper contribution is a new experimental environment where every parameter is monitored and automatically recorded, for example, precise robotic control of previously hard-to-quantify parameters such as antisolvent dispensing during spin coating [13]. Machine learning cannot compensate for poor experimental data: uncontrolled variation between nominally identical runs is noise that can obscure real correlations, while reproducible robotic execution turns each run into a well-defined data point.

Recent reviews make the same point: Chen et al. note that AI's predictive reliability is limited by patchy, low-reproducibility manual data [14], and Lee et al. describe automation as key to systematically exploring the highly coupled parameter space of perovskite solar cells [15].

Robotics is therefore best understood not as a source of speed, but as the infrastructure that makes experimental data trustworthy enough for machine learning to be genuinely useful.

2. The Transformation of Research Approach

Robotics' most transformative contribution is not only automation, but precision, reproducibility and completeness of record beyond what is realistic in a human-operated laboratory.

Take spin coating: nominally identical recipes still vary in timing, dispensing and thermal history in ways too small to control by hand but large enough to affect film formation and device performance, especially in quenching-sensitive systems. Detailed process-dynamics modelling confirms just how sensitive film formation is to exactly these small execution differences [16].

A robot instead executes and logs the recipe as a precisely time-stamped sequence, turning each device into data accompanied by a complete, machine-readable processing history. Automation removes operator-dependent variability, but it does not by itself guarantee reproducibility. Batch-to-batch variation in precursor materials, differences in device-testing protocols and environmental conditions such as humidity and temperature can all still introduce inconsistency and each must be controlled and monitored independently of the robotic execution itself. Machine learning is only as useful as the data it learns from: uncontrolled variation between nominally identical experiments is noise that can obscure or fabricate correlations, even for sophisticated algorithms. Robotic experimentation offers a way out, transforming data from isolated results into a structured, reproducible process–structure–property dataset (Figure 1).

Standardised workflows can also support FAIR data principles—Findable, Accessible, Interoperable and Reusable—provided that appropriate metadata standards and data-sharing practices are adopted. The researcher remains responsible for defining the scientifically meaningful search space, for example candidate chemistries, solvent systems and annealing routines, within which the algorithm selects informative experiments [17].

This also breaks the one-factor-at-a-time habit: rather than isolating each parameter in turn, a designed experimental matrix explores several jointly, revealing interactions a sequential approach would miss.

Because every experiment is executed under tightly controlled, fully recorded conditions, machine learning can then propose the next most informative experiment rather than the researcher guessing which parameter to try next.

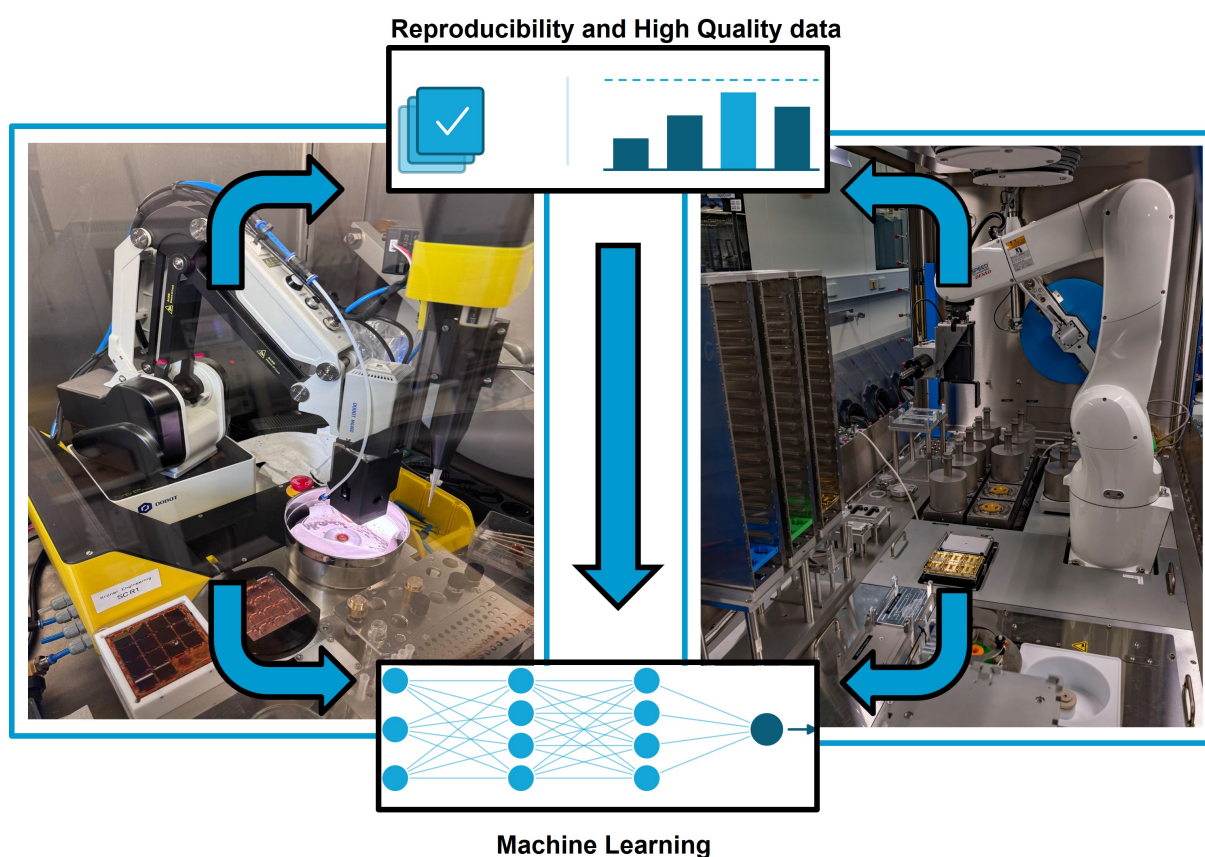


Figure 1. Robotics provides the reproducibility that turns experiments into high-quality data, which machine learning uses to design the next, more informative experiment. (**Left:** robotic platform of the Schmidt-Mende group, University of Konstanz. **Right:** robotic platform of the Bach group, Monash University. Both photographs are original and unpublished, provided by the respective co-authors).

This reproducible, information-rich data also enables a shift from optimizing one metric to several simultaneously (see Table 1), since the highest-efficiency device is not always the most valuable one once lifetime, stability, and resource use are considered.

Table 1. Traditional optimization vs. autonomous multi-objective optimization.

Traditional Optimization	Autonomous Multi-Objective Optimization
Maximize power-conversion efficiency (PCE)	Optimize PCE together with stability, lifetime, reproducibility, and sustainability
One primary target	Multiple objectives optimized simultaneously
Optimize parameters sequentially	Explore multidimensional parameter spaces
One-factor-at-a-time experiments	Design of experiments and systematic parameter matrices
Researcher-defined experimental space and human-chosen next experiment	Machine-learning-guided experiment selection within a researcher-defined experimental space
Researcher-specific, variably structured data and incomplete metadata	Standardised, structured data and metadata that enable comparison, sharing and reuse
Optimize the best-performing device	Identify robust and Pareto-optimal processing windows
Performance-focused	Performance + durability + resource efficiency + environmental impact
Minimize experiments manually	Maximize information gained per experiment

A robotic, ML-driven laboratory can pursue these objectives directly, asking not simply which process is most efficient, but which combination of materials and conditions gives the best overall performance. We draw

this contrast for clarity, not as a strict rule. Design of experiments, structured data collection and multi-objective thinking already appear in many conventional, non-autonomous workflows too. Automated platforms themselves vary widely as well, from simple robots that just carry out a researcher's fixed protocol, to fully closed-loop systems where machine learning chooses the next experiment on its own. So the distinction we draw in this Perspective is a matter of degree: how much of the design and interpretation work is carried by the researcher versus by the system, not a sharp line between the two. None of this makes the researcher unnecessary. As operator-dependent variability is designed out of the fabrication step, the value a researcher adds shifts location rather than disappearing: away from manually executing and fine-tuning individual runs and towards decisions a robot or algorithm cannot make on its own. This includes defining the experimental space and the chemistries or process windows worth exploring in the first place, choosing which objectives to weigh against each other, judging whether a proposed characterization metric is actually measuring what it claims to measure, recognising when an algorithm's suggestion reflects a real physical mechanism rather than a dataset artefact and deciding when a surprising result warrants manual follow-up rather than being accepted at face value. Automation does not remove the researcher from the loop; it moves their expertise upstream, from executing experiments to designing and interrogating the system that runs them.

3. A Case Study: Automating a Perovskite Processing Step

In our own laboratory, this shift has already been demonstrated in practice, not merely proposed as an aspiration. We use a robotic platform shown in (Figure 1) to automate a key film-formation step in perovskite fabrication, executing it identically on every run across a fully recorded set of parameters. We initially optimized the gas-quenching process manually [18–20], which exposed the limits of manual spin coating: gas quenching is highly sensitive to the geometry of the gas flow, in ways that are difficult to control reliably by hand but well suited to precise robotic control. Simply using a robot to repeat a fixed process, however, is not enough on its own. The real advantage comes from combining it with statistical approaches such as design of experiments (DoE) and machine learning. We offer this only as an illustration of the kind of insight such a workflow makes accessible, isolating variables that would otherwise be inseparable from ordinary operator variability and exploring several jointly rather than one at a time and not as evidence supporting the general claims made elsewhere in this Perspective. The specific findings are unpublished, remain the subject of a separate manuscript in preparation, and are not reported here.

The broader point holds regardless of process: a robotic platform's real contribution is experiments precise enough that their differences can be trusted to reflect the parameters under study, not how each run happened to be carried out. Perovskite photovoltaics is used as the illustrative case throughout this Perspective, but the argument is not specific to this material system: the reproducibility challenges and the way data are produced and handled, are largely the same across perovskite and organic photovoltaics. Organic photovoltaic devices are comparably sensitive to processing history and automated, robot-based platforms combined with machine learning are already addressing this in that field: one such platform screened around 100 processing conditions and reported a power-conversion-efficiency standard deviation below 0.2% across 36 identically processed devices, with reproducibility maintained over several months [3], and a follow-up study applied the same automated approach across more than 40 donor–acceptor combinations to map how processing conditions affect operational stability [21].

4. Analyzing Data Is Harder Than Getting Data

Robotic execution solves half the reproducibility problem: producing the data. It does not solve the other half: knowing which parameter to measure and which tool to measure it with. Processing alone does not guarantee quality: a thoughtful approach to analyzing the data and understanding what it actually shows, matters just as much. Selecting an appropriate model for the data at hand and checking that choice against reasonable alternatives, is essential; cross-validation, often skipped in machine learning papers, is one simple but easily overlooked part of that process. With the small, expensive-to-generate datasets typical of experimental materials science, an overly complex model can fit noise as readily as signal, making that validation step even more important, not less.

Even with automation, however, experimental materials datasets remain sparse relative to the dimensionality of accessible chemical and processing spaces. Higher throughput improves data quality and quantity but cannot exhaust these spaces. Adaptive decision-making is therefore needed to maximise the information gained from every experiment.

Different kinds of analysis raise their own, distinct problems. In image analysis, for instance, standard tools carry their own assumptions: Otsu's thresholding [22] is used to separate foreground and background and tends to perform best when their intensity distributions are clearly separable. However, this condition does not always hold, and the method still returns a threshold that is optimal according to its criterion, even when the resulting segmentation may be unreliable. In our experience, an automated metric is only as trustworthy as its validation against independent, human-judged ground truth. That validation cannot stop after one check, since a metric that

passes on one dataset can still fail silently on another. This is not a hypothetical risk: a recent machine-learning model for perovskite solar cell performance reported within-laboratory R^2 values as high as 0.44, yet collapsed to leave-one-laboratory-out R^2 values as low as -3.05 once tested across different labs: the model had learned laboratory-specific processing signatures rather than a transferable composition-efficiency relationship, and its strong within-dataset validation gave false confidence in its broader applicability [23]. A metric worth keeping must also earn its place: one that is redundant with another, or that correlates with the outcome of interest in the wrong direction, is better dropped than kept for the sake of having more numbers to report.

This is not unique to organic and perovskite photovoltaics. Automated-characterization pipelines elsewhere in materials science report the same need for independent validation [24]. The multi-objective optimization argued for above (Table 1) is only as sound as the metrics that feed it: a robotic laboratory can make experiments reproducible, but it cannot by itself make a characterization metric meaningful.

5. Conclusions

Robotic fabrication, on its own, only solves part of the problem: it makes experiments precise and reproducible enough to trust. Turning that data into progress still depends on choosing the right models, metrics, and objectives, validating against independent evidence.

Machine learning is what closes the loop. Instead of varying one parameter at a time, it can explore multidimensional spaces, weight efficiency against stability, reproducibility and resource use simultaneously, and surface interactions a sequential search would never find.

This shifts the role of researchers away from manually tuning parameters and towards framing the right questions, designing the experimental space and judging the resulting numbers.

For perovskite and organic photovoltaics, this could mark the transition from trial-and-error optimization toward reproducible, data-rich, closed-loop exploration of multidimensional processing spaces. Every experiment would then contribute not only to the fabrication of another solar cell, but also to a growing quantitative understanding of how materials, processing conditions, structure, and device properties are interconnected. We strongly believe that we will see for the future of perovskite and organic solar cell research a transformation towards robotic processing and the usage of machine learning for finding correlations and improved understanding of the role of processing parameters.

Author Contributions

M.A.: conceptualization, original draft writing, visualization, reviewing and editing; S.K.: reviewing and editing; N.C.: reviewing and editing; N.F.: reviewing and editing; L.S.-M.: conceptualization, reviewing and editing, supervision; U.B.: conceptualization, reviewing and editing. All authors have read and agreed to the published version of the manuscript

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Conflicts of Interest

Given the role as Editor-in-Chief, L.S.-M. had no involvement in the peer review of this paper and had no access to information regarding its peer-review process. Full responsibility for the editorial process of this paper was delegated to another editor of the journal. The other authors declare no conflict of interest.

Use of AI and AI-Assisted Technologies

During the preparation of this work, the authors used ChatGPT (OpenAI) to discuss aspects of the work, generate ideas, and improve the language and readability of the manuscript. After using this tool, the authors reviewed and edited the content as needed and take full responsibility for the content of the published article.

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