Fundamental advances to increase the efficiency as well as stability of organic photovoltaics (OPVs) are achieved by designing ternary blends, which represents a clear trend toward multicomponent active layer blends. The development of high-throughput and autonomous experimentation methods is reported for the effective optimization of multicomponent polymer blends for OPVs. A method for automated film formation enabling the fabrication of up to 6048 films per day is introduced. Equipping this automated experimentation platform with a Bayesian optimization, a self-driving laboratory is constructed that autonomously evaluates measurements to design and execute the next experiments. To demonstrate the potential of these methods, a 4D parameter space of quaternary OPV blends is mapped and optimized for photostability. While with conventional approaches, roughly 100 mg of material would be necessary, the robot-based platform can screen 2000 combinations with less than 10 mg, and machine-learning-enabled autonomous experimentation identifies stable compositions with less than 1 mg.

With the development of novel nonfullerene acceptors fundamental performance limitations of fullerene-based organic solar cells (OSCs) have been overcome. In the currently highest performing system PM6:Y6 ternary additives are used to improve charge carrier lifetime and mobility resulting in significantly improved performance with efficiencies up to 16.5%. Typically in ternary systems the host donor:acceptor (D:A) ratio is kept constant, while only the content of additive is varied due to limited experimental resources. The existence of other optima beyond these constraints is usually not investigated. On the other hand, also for improvements of stability, ternary additives have successfully been introduced to stabilize morphology or prevent oxidation. These desired effects of additives are typically reverted into detrimental effects depending on the concentration and compatibility of the additive with the host system. Finding a fine balance is necessary to determine if a given additive can lead to a performance enhancement for a given host system. Currently the Achilles heel of the highest performing organic photovoltaic (OPV) systems is device stability, which motivates the use of a fourth stabilizing additive in performance optimized ternary systems. On the pathway to such highly complex optimization problems with multidimensional composition space and hundreds of possible candidates for performance enhancing additives, novel experimental methods are necessary.

High-throughput experimentation (HTE) addresses these challenges by assisting the researcher in material synthesis, sample processing, and characterization. High-throughput methods for polymer samples have been used for adhesion...
evaluations\(^{[6]}\) and cell biology research.\(^{[7,8]}\) To the best of our knowledge, the first robotic setup for combinatorial research in organic electronics was introduced by Kiy et al. including film fabrication via spin-coating and various characterization tools.\(^{[9]}\) One of the main challenges of combinatorial research in OPV is the scalable fabrication of high-quality individual films. Recent approaches are based on gradient coating or ink-jet printing, which are usually limited by the number of mixable components, the number of samples, or the need for specific ink properties.\(^{[10–12]}\) An HTE coating method for organic semiconductors with a scalable number of mixable components and scalable number of films is not yet established. Therefore, we introduce a robot-based production of OPV-films via drop-casting that can mix a large number of components to form up to 6048 films of different compositions per day.

Applying this HTE system allows the screening of such a vast number of compositions containing hundreds of possible components that conventional experimental planning and evaluation capabilities are exceeded. Therefore, as a second approach, we combine our HTE production line with a machine learning (ML) tool\(^{[13–16]}\) to form a self-driving laboratory (SDL), for accelerated process optimization and materials discovery.

In this ML-driven approach, new experiments are suggested based on all previously collected measurements. To this end, the ML decision-maker infers the outcomes of all possible experiments, leveraging statistical correlations identified from the prior measurements, and suggests the most informative ones for future evaluation.

To the best of our knowledge, the first self-driving laboratory reported an autonomous chemical synthesis where all the steps of the experimental procedure are controlled by a computer and driven by a local optimization algorithm.\(^{[17]}\) Since then, the self-driving approach was used to optimize carbon nanotube growth,\(^{[18]}\) polyanionate clusters, metal-based alloys,\(^{[19]}\) and organic synthesis reactions.\(^{[20,21]}\) More recently, in an area related to this work, a thin-film self-driving robot was used to improve film quality and thermal stability of hole-transport materials for clean energy technologies.\(^{[22]}\)

Herein we demonstrate the benefits of HTE and the self-driving approach on the design of photostable material composites for OPV. While recently lifetimes of up to 10–20 years under continuous illumination in nitrogen atmosphere were reported,\(^{[23–25]}\) photostability of OSC materials under the influence of oxygen and moisture is a critical challenge. Currently available encapsulation films for OPV materials are a major cost factor of the final product while their water vapor transmission rate is typically 10\(^{-3}\) g (m\(^2\) day\(^{-1}\)). As higher quality barrier films are currently not manufacturable at a competitive price, optimizing active layer materials for photostability in the presence of oxygen and water is a critical step for commercial applications. Interestingly, complex photochemical interactions between donor, acceptor and oxygen can suppress or enhance photooxidation in D:A blends.\(^{[26,27]}\) Further, adding a third component to the active layer may increase thermal and light stability.\(^{[28,29]}\) However, the degradation behaviors of higher dimensional multicomponent systems may depend on various interactions between the components.

Therefore, we use an optimization of four component active layer blends as an experimental proof of concept for our high-throughput film formation and characterization system with machine-learning-enabled self-driving capability. In the following, grid-based high-throughput experimentation will be compared to the self-driving approach (Figure 1C).

The automated platform (Figure 1B; Figure S1, Supporting Information) employed for this study was already used in our group to successfully synthesize and characterize organo-metal-halide perovskites and organic nanoparticles with outstanding precision.\(^{[30,31]}\) To form high quality drop-cast films on inert carriers, we optimized a system to create separate wells on a glass plate. Printing a well structure with UV-curable epoxy allowed a minimal height of the separating walls to reduce material accumulation at the walls resulting in high quality films with a large homogenous area (Figure 1C; Figure S2A, Supporting Information). Demonstrating the scalability of our approach, two quaternary blend systems were investigated simultaneously.

In the first system, the poly(3-hexylthiophene-2,5-diyl)(6,6)-phenyl-C61-butyric acid methyl ester) (P3HT:PCBM) reference is blended with rhodanine-benzothiadiazole-coupled indacenodithiophene (IDTBR), a stable nonfullerene acceptor as well as poly[4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)benzo[1,2-b;4,5-b]dithiophene-2,6-diyl-alt-(4-(2-ethylhexyl)-3-fluorothieno[3,4-b]thiophene-2-carboxylate-2,6-diyl)] (PTB7-Th), an instable polymer donor (white squares in Figure 1A). In the second system a benzodithiophene-quinoxaline based copolymer (PBQ-QF), a versatile donor that works with most acceptors, is used (black squares in Figure 1A). All materials are readily available in large quantities and well-studied allowing extensive tests with simple verification. Overall for both material systems, almost 2100 single films were fabricated and tested within 7 d with more than 5000 recorded absorbance spectra, see experimental section and Figure S2B in the Supporting Information.

In Figure 1C, the experimental workflow of the robot process is illustrated schematically. Starting with a predefined grid of compositions (or the ML-self-driving approach), individual inks are formulated automatically using a commercially available liquid-handling robot. The inks are drop-cast onto customized 96-well glass substrates to form uniform semiconductor layers. The glass plates are then illuminated with metal halide lamps at one sun intensity for 18 h in ambient air to induce photooxidation of the active layers, which can be measured by absorbance loss. Absorbance spectra were recorded before and after light treatment using a microplate reader.

The reproducibility of film formation and degradation is very high with an R\(^2\) of 0.97 for 309 tested samples (Figure S3, Supporting Information) while the film thickness, as measured by a profilometer, ranged between 70 and 80 nm. Given the accuracy of our dispensing system, we allowed variations of all four components (PTB7-Th, P3HT, IDTBR, PCBM) in two percent formation. Demonstrating the scalability of our approach, two quaternary blend systems were investigated simultaneously.

The first high-throughput test, a subset of 1041 points was selected containing all single components, binary and ternary variations with 10 wt% increment (202 samples) as well as 820 randomly selected quaternary samples plus 19 duplicates for reproducibility verification. For the second system, the same set of compositions was used while only PTB7-Th was replaced by PBQ-QF.

The degradation behavior of the quaternary system containing PTB7-Th is depicted in Figure 2A (left side) where degradation is denoted as the integral change of the absorption
spectra for each composition before and after degradation. It clearly shows strong degradation of PTB7-Th with a relative absorbance loss of 68%, while P3HT lost around 19%. The two acceptor materials exhibited minimal change in absorbance. Moreover, it is observed that the binary series of PTB7-Th toward PCBM or oIDTBR (see also Figures S4 and S5 in the Supporting Information) leads to a linear increase of photostability with acceptor content. But non-linear trends are observed as well, as already slight amounts of P3HT (≈10 wt%) stabilize PTB7-Th completely leading to blend stabilities similar to pristine P3HT. More surprisingly, blends containing both oIDTBR and PCBM show a drastic destabilization effect causing a large unstable area in the quaternary space (Figure 2A). As this is also observed in a binary mixture of PCBM and oIDTBR (absorbance loss up to 74%) it seems to be caused by a specific interaction between the two acceptors that may be rooted in the formation of mixed phases with a composition that is more susceptible to photooxidation processes. In the second quaternary system, where PTB7-Th is replaced with PBQ-QF, the same PCBM:oIDTBR instability area is discovered, while most other compositions show improved photostabilities, which is in line with the high stability of pristine PBQ-QF (Figures S4–S6, Supporting Information). A detailed viewing of the robot process and the 4D stability-space is found as cinematic illustration in the supporting information. These results of our lab scale high-throughput film formation technique enable a valuable screening method for interactions in complex multicomponent blends. However, for the stability of final OPV products additional interactions with interface materials and electrodes as well as variations of morphology due to different coating techniques will have to be considered.

Instead of a large predefined grid, we utilized intelligent experimental design for the self-driving approach (SDA). The machine learning driven software package ChemOS coordinates the flow of information between the automated equipment, the researchers and the experiment planning module. The software enables the remote exchange of experimental parameters and measurements, which enables the operation of experiment planning strategies and robotics platforms at different locations. In line with the identified steps of closed-loop experimentation, we extended ChemOS by an additional module which maps the parameter space of the experiment planner to technical constraints of the robot (see Section S1 in the Supporting Information).

From the experiment planner, we used the active learning global optimizer Phoenics to learn and navigate the multidimensional parameter space. This ML strategy learns by doing and does not need to be trained with prior measurements. Following a Bayesian optimization strategy, a surrogate model is constructed from parameter kernel densities estimated via Bayesian neural networks. This architecture enables a favorable linear scaling and reduces the computational cost of the
optimization algorithm in contrast to, for example, approaches based on Gaussian processes. Phoenoics also streamlines the throughput of automated solutions via a sampling parameter, which explicitly controls the sampling behavior of the algorithm, gradually exploring and exploiting. Alternating the sampling behavior during the experimental campaign has been shown to accelerate the optimization process and reduce the number of samples. In this experiment, ChemOS leveraged Phoenoics to suggest four blends per closed-loop event, and increases the experimentation throughput by simultaneously coordinating the self-driving approach for the two studied blend systems. To ensure that any active layer composition which will be found contains an OPV relevant donor:acceptor ratio, a boundary condition limits the D:A ratio from 1:5 to 5:1. Starting from four random compositions and their stability results, ChemOS iteratively suggested the next set of four compositions which were fabricated, degraded and characterized. As an initial test run 15 iterations requiring 15 consecutive 18 h degradation tests were made. Here, two identical samples were fabricated for each composition to probe experimental noise.

While the SDA focused more on the stable regions in an exploitative search toward a global minimum an explorative component probed numerous stable and unstable compositions covering largely the same experimental space as the high-throughput test. The experimental space for both HTE and SDA in the PTB7-Th-based system is displayed in Figure 2B (for PBQ-QF see Figure S7 in the Supporting Information). Here, each data point represents the stability of a quaternary composition plotted over their distance (in terms of compositional difference) to the most stable composition as found by grid-HTE. The results demonstrate how the Bayesian optimization reconstructed the stability distribution of grid-HTE with a much smaller number of samples (only 7%) compared to HTE. Generally, photostable compounds can be found along the entire distance axis, indicating a broad area of stable compositions rather than a single point minimum (Figure S8, Supporting Information). To accommodate for such broad minima, the merit function had been adjusted after an initial test run (see the Supporting Information ). It is observed that the self-driving approach is able to find competitive photostable blends within only 15 learning iterations (four samples each). The best compositions found by the two formulated merit functions are on a par with the best compositions screened by grid-HTE (Table S1 in the Supporting Information).

To have a large number of tests that allow statistical comparisons between HTE and SDA, virtual experiments were performed on a calculated stability grid. From the data collected for the two blend systems during the HTE runs, we constructed probabilistic regression models to emulate the response surfaces of the two experiments (Figure 2A; Figure S5, Supporting Information). Then models, or virtual robots, were set up as Bayesian neural networks (BNNs) and were trained to predict the photostability for any possible set of material compositions for the two blend systems. This approach has already been demonstrated in the context of emulating HPLC calibrations. Details on the network architectures, the training procedures and the prediction accuracies on the observed (training sets) and unobserved data (test sets) for both blends are reported in the supporting information (see Section S3 in the Supporting Information). The virtual robots and the complete set of experimental data are made available on GitHub.

Our results on the virtual robots (Figure 3A) indicate that the self-driving approach requires on average 27 samples on the PTB7-Th blend system to identify a blend which is at least as photostable as the most stable blend discovered by grid-HTE. Furthermore, we find that within a given budget of 30 (60) samples, the SDA identifies more photostable blends than HTE with a chance of about 96% (97.5%) (Figure 3B). Based on these results the discovery of photostable blends is accelerated by a factor of ~33× for PTB7-Th (and ~32× for PBQ-QF; Figure S9 in the Supporting Information) over conventional HTE as indicated by the virtual robots. Further details on the statistical analysis are reported in the ESI (see Section S4 in the Supporting Information).

Figure 3C demonstrates the benefits of grid-based high-throughput research and the self-driving approach over manual experimentation. Within this comparison we assume that systematic manual testing requires the preparation of 500 samples, with a throughput of 20 samples per day, to obtain equivalent information as with HTE of 1000 samples. Using conventional 1-in. substrates, typical solution concentrations of 30 mg mL−1 and coating methods, such as spin-coating or blade-coating, a consumption of 188 mg per compound is expected. In contrast, HTE needs only 7.5 mg per compound due to the low...
Figure 3. A) Performances of high-throughput experimentation (red traces) and ChemOS/Phoenix (blue traces) on the virtual robots related to the PTB7-Th-based system. Note that the traces were averaged over 10000 independent grid samplings and 200 independent ChemOS optimizations. B) Top: Statistical output of the virtual robot showing the acceleration of SDA over HTE. Bottom: Confidence to improve on HTE within given budget of 30 or 60 samples. Both are related to the PTB7-Th-based system. C) Consumption comparison between manual testing, high-throughput experimentation, SDA with budget of 60 samples and virtually optimized SDA with budget of 30 samples. The calculations are limited to one quaternary system.

Experimental Section

High-Throughput Coating: Stock solutions of the materials in chlorobenzene were manually prepared with a concentration of 0.6 mg mL\(^{-1}\). All further ink formulations were mixed by a liquid handling robot [Freedom Evo 100; Tecan Group AG, Switzerland] using 96-well polypropylene microplates [Eppendorf, Germany]. To guarantee good intermixing, an aspirate/dispense step was repeated for three times before drop-casting 25 µL of each mixture onto a pre-patterned glass substrate. The films are dried at 60 °C for 4 min. 96 individual films can be formed in 22 min. To obtain stable morphologies, a thermal annealing step at 120 °C for 15 min was performed. Further descriptions are reported in the supporting information (see Section S5 in the Supporting Information).

Supporting Information

Supporting Information is available from the Wiley Online Library or from the author.

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| Photo-stability [arb. unit] | # Samples | Average acceleration over HTE | Probability to find more photostable blend than HTE [%] |
|---------------------------|-----------|-------------------------------|-----------------------------------------------|
| 0.96                      | 30        | 40                            | >95                                           |
| 0.94                      | 60        | 30                            | >95                                           |

| mg per ingredient | Material | Samples per day | Throughput | Duration |
|-------------------|----------|-----------------|------------|----------|
| 0.1               |          | 10              | 5          | 10       |
| 1                 |          | 10              | 2          | 20       |

Concentration of 0.6 mg mL\(^{-1}\) used in drop-casting. Moreover, even as 288 samples are tested in a single day, HTE guarantees a stable process with highly reproducible data. The substantially reduced number of samples for the self-driving approach with only 60 samples further reduces the amount of consumed materials to 0.45 mg per compound. Following the findings from the virtual robots, the number of samples could even be reduced to 30 (0.225 mg) while maintaining a confidence of over 95% (optimized SDA). Note that for ChemOS the given throughput of four samples per day and blend system is based on the iterative degradation process. Nevertheless by parallelization across blend systems, ChemOS is able to run and optimize 16 blend systems simultaneously further accelerating the discovery process.

We have demonstrated how complex multicomponent optimization problems for next generation OSC active layers can be highly accelerated by a novel high-throughput film deposition technique combined with automated characterization and machine-learning-enabled experimental design. Over 2000 different quaternary active layers were tested in 7 d with a materials consumption of less than 15 mg per component. This enables a more thorough stability investigation of novel OPV materials and their interactions with other blend components at ultralow material consumptions. Implementing a machine learning optimization algorithm, equivalent information about stability minima and maxima could be found with a sample reduction of around 93%. In our specific test case, P3HT and PBQ-QF rich blends show improved stability over PTB7-Th rich blends. O-IDTBR and PCBM can destabilize each other with dramatic consequences for the active layer blend.

As a next step the inclusion of additional characterization methods and target properties, e.g., photoluminescence or conductivity, could allow not only optimization for stability but also for electrical performance. Recently, Häse et al. with Chimera, demonstrated a hierarchy-based general purpose achievement scalarizing function designed to address multiparameter optimizations in self-driving laboratories.[35]
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Conflict of Interest
The authors declare no conflict of interest.

Author Contributions
S.L. and F.H. contributed equally to this work. C.J.B., T.H., and A.A.-G. conceived and supervised the project. S.L. developed the substrate patterning and optimized the robot-process. F.H. and J.D.P. performed the experiments. S.L. evaluated the data and interpreted the experimental results. F.H. and L.M.R designed and implemented the virtual robot, which were implemented and executed by ChemOS. F.H. and L.M.R designed statistical analyses and self-driving laboratories optimize multi-component systems.

Keywords
high-throughput experimentation, machine learning, organic photovoltaics, photostability, solar energy

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