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# A Helping Hand: A Survey About AI-Driven Experimental Design for Accelerating Scientific Research

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**Abstract:** Designing and conducting experiments is a fundamental process across various scientific disciplines, such as materials science, biology, medicine, and chemistry. However, experimental research still predominantly relies on traditional, time-consuming, resource-intensive, and costly trial-and-error experimentation approaches that hinder rapid discovery, reproducibility, and scalability. Recent advances in artificial intelligence (AI) and machine learning (ML) offer promising alternatives, but a comprehensive overview of their implementations in experimental design is lacking. This research fills this gap by providing a structured overview and analysis of existing frameworks for AI-driven experimental design, supporting researchers in selecting and developing suitable AI-driven approaches to automate and accelerate their experimental research. Moreover, it discusses the current limitations and challenges of AI techniques and ethical issues related to AI-driven experimental design frameworks. A search and filter strategy is developed and applied to appropriate databases with the objective of identifying the relevant literature. Here, active learning, particularly Bayesian optimization, stands out as the predominantly used methodology. The majority of frameworks are partially autonomous, while fully autonomous frameworks are underrepresented. However, more research is needed in the field of AI-driven experimental design due to the low number of relevant papers obtained.

**Keywords:** AI-driven; experimental design; autonomous; optimization; active learning



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## 1. Introduction

In recent years, the integration of artificial intelligence (AI) into real-world applications has gained significant attention, especially after the introduction of large language models (LLMs) such as ChatGPT4, which have demonstrated capabilities in natural language understanding, rapid data analysis, and knowledge synthesis. These advancements reflect a broader trend: AI systems are increasingly capable of supporting complex cognitive and decision-making tasks across diverse domains [1]. This trend has also found its way into scientific research, where AI is not only used for data analysis and modeling but is also beginning to reshape how experiments are designed and conducted [2].

Traditionally, scientific experimentation, particularly in fields such as biology, chemistry, and materials science, has relied on human intuition and iterative, time-consuming trial-and-error processes [3]. In such domains, selecting the right experimental parameters from a vast and multidimensional space is a major challenge, often limiting the pace and scope of discovery.

Leveraging AI for experimental design offers outstanding advantages over this method of human-based experimentation. AI can model complex relationships between parameters and outcomes, propose efficient experimental strategies and continuously improve by

learning from previous results. A sketch of the AI-driven experimental design workflow can be found in Figure 1.

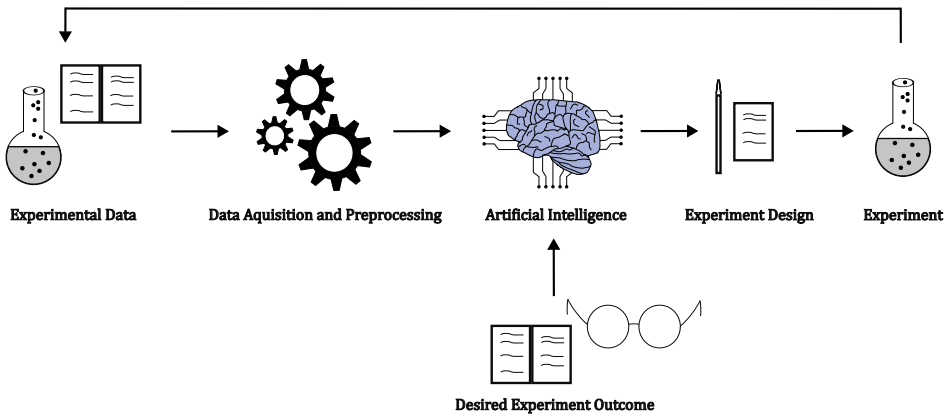


**Figure 1.** Schematic illustration of the AI-driven experimental design workflow. Available experimental data are used to train AI. The scientist defines an experimental objective, and AI suggests experimental designs to the scientist accordingly or performs them autonomously.

As a result, experiments can be performed precisely and efficiently, saving time and material by avoiding unnecessary trials. Consequently, there are reductions in cost for both experiments and potentially environmentally hazardous waste. In combination with an autonomous platform incorporating an experimentation and analysis stage, experiments can be performed autonomously. This concept is referred to in the literature as a "self-driven laboratory" (SDL) [4]. The autonomous execution and analysis of experiments further enhance the reproducibility of experiments and continuous experimentation, ideally operating without the need for human intervention. SDLs for different applications have been reported [2,4–14].

The literature incorporates various reviews highlighting the role of AI in accelerating scientific research across diverse fields with a particular focus on AI-driven experimental design [2–13,15–17]. Some reviews related to AI-driven experimental design target a specific domain, such as organic/inorganic semiconductors (materials science) or drug formulation (medicine), providing architectures or frameworks that are intended to be applied in the addressed field. Others concentrate on a specific technique, such as LLMs. The majority of reviews focus on self-driving laboratories rather than AI–human frameworks. Currently, the literature lacks a cross-domain perspective and merely provides general overviews and analyses of existing frameworks for AI-driven experimental design across different domains. Thus, an outline of applied AI methodologies in experimental design is missing. Furthermore, previous reviews overlook key aspects such as the degree of automation, online capability, and generalizability of AI frameworks.

In contrast, this study highlights the current state of AI-driven experimental design by analyzing existing approaches and frameworks. This encompasses both the AI techniques used in experimental design and the applied frameworks in general. In terms of a generic analysis of the framework, different aspects are considered. This includes the scientific domain, the degree of automation, the kind of data, and online and generalization capabilities. Additionally, the limitations and challenges of current AI methodologies, as well as explainability and ethical issues, are considered and discussed. By analyzing the existing literature accordingly, this research aims to guide researchers in identifying an ideal AI-driven experimental design system to accelerate their experimentation processes and, thus, their scientific research.

This study is structured as follows. The first part explains the methodology of the research, incorporating the search and filter strategy as well as the used taxonomy to guide the investigation of the filtered contributions. The second part covers the results and provides a discussion, while the third part concludes with the findings of this study.

## 2. Methodology

This section outlines the methodology used to conduct the systematic literature review of AI-driven experimental design. A search strategy is developed to clearly define the scope of this study. Relevant scientific databases are selected and queried using a carefully designed search query. Appropriate filters are applied to ensure the inclusion of only relevant publications while excluding non-relevant ones. The resulting set of contributions is then investigated using a well-defined taxonomy, leading to a structured and consistent analysis of the included studies. A sketch of the applied methodology can be found in Figure 2.

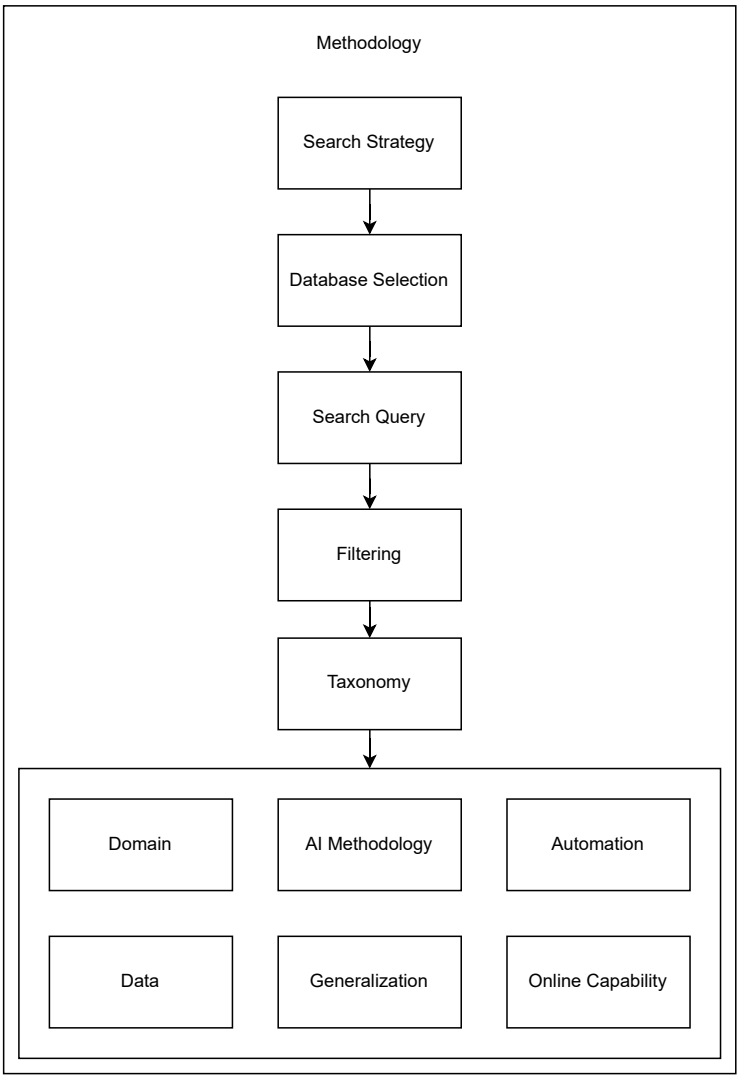


**Figure 2.** Schematic illustration of the applied methodology.

### 2.1. Search Strategy

To efficiently guide this study's research toward the desired search space and exclude non-relevant publications, the subsequent search strategy is applied. It follows Piliuk and Tomforde [1] and encompasses the following steps:

1. Define research questions for guiding the systematic research.
2. Create an appropriate search query by defining meaningful search terms and assessing relevant databases.
3. Determine filter criteria to exclude non-relevant studies.
4. Apply the filter criteria through appropriate procedures.

To guide the literature research of this study, the following research questions are defined:

1. In which research fields and kinds of applications are AI techniques used to automate experimental design?
2. Which quantitative methods are used to implement AI in experimental design?
3. Which tasks in the experimental design process are addressed by these techniques?
4. What kind of data are used?
5. Are the proposed frameworks online-capable, and can they generalize well to new data?

The first question aims to identify the fields and applications in which AI-driven experimental design is applied. The second question aims to investigate which AI methodology is employed to ensure that the scope of the research lies within AI-driven experimental design. The objective of the third question is to examine which experimental design tasks within the experimental design process are addressed using AI methodologies. The fourth question addresses the data utilized, while the fifth question aims to analyze the online and generalization capabilities of the proposed frameworks. The publications included in this research are intended to answer these questions in order to provide a comprehensive overview of AI-driven experimental design. Thus, this study investigates various databases to ensure a comprehensive and balanced review of the existing literature, covering both method-specific and subject-specific resources.

Databases typically accepted in the field of AI, such as the ACM Digital Library and IEEE Xplore, are included. Additionally, subject-specific and experimental design-related resources, like ACS Publications and RSC Publishing, which focus on biology, chemistry, and materials science, are examined. To incorporate medicine-related publications, PubMed is also considered. Furthermore, general databases, including ScienceDirect and SpringerLink, are utilized to broaden the scope of the research. This selection of databases—two focused on AI, two on materials science, biology, and chemistry, one on medicine and biology, and two general repositories—ensures a broad and diverse overview of the relevant literature regarding AI-driven experimental design, balancing method-specific resources of AI research with subject-specific studies in experimental design while disregarding those with a very limited application focus or low popularity.

The assessed databases are queried by applying an appropriate search query. It combines various meaningful search terms. Using a search query ensures the reproducibility of our research. For this work, a search query is experimentally derived, and the following combinations of search terms were found to yield the best results for relevant studies: *"artificial intelligence" AND "driven" AND ("experiment planning" OR "experiment selection" OR "experiment parameter adaption")*. The first part of the query ("artificial intelligence" and "driven") narrowed the search to publications that apply AI methodologies. Thus, the authors of this research could focus on intelligent, automated solutions and omit manual, hand-optimized approaches. During the development of the search query, it was found that using the term "artificial intelligence" consistently included all relevant publications identified in this study. In contrast, replacing it or adding other terms, such as "machine learning", "deep learning", or "automation", either excluded relevant studies or significantly increased the inclusion of non-relevant publications. Therefore, "artificial intelligence" was retained as the primary term to ensure both coverage and precision in the

literature search. The same development and trade-off strategy was applied to the other terms in the final search query.

The second part ensured that the scope of the contributions included experimental design and, therefore, set appropriate research boundaries. Thus, terms typically related to the experimental design process were identified and used accordingly. By applying the mentioned search query to the aforementioned databases, a well-functioning trade-off between obtaining less relevant contributions and too many non-relevant publications was achieved.

The proposed search strategy resulted in 329 contributions. Consequently, the search space was set to the period from 2000 to 2025, which led to the exclusion of 61 contributions. In addition, duplicate publications, which occurred in multiple databases, covering 14 publications and 20 non-research-based results, such as tables of contents, lists of references, or whole proceedings, were removed. Thus, 234 contributions were obtained and further investigated.

### 2.2. Filtering

This section discusses the filtering of relevant publications from the pool of contributions obtained by applying the aforementioned search query. Several filter criteria (FC) were applied to obtain the relevant publications that addressed the defined research questions and excluded the non-relevant ones.

First, to ensure a focus on concrete AI-driven experimental design solutions with corresponding results, the scope of relevant studies was limited, disregarding preliminary concepts and ideas. Thus, reviews, abstracts, concept papers, pre-prints, etc., were excluded (FC1). In addition, papers that did not propose quantitative AI-based methodologies but instead focused solely on statistical methods without a learning component were excluded (FC2). Furthermore, papers that failed to provide a clear explanation of the quantitative algorithms employed were also filtered out.

Apart from that, all studies that did not focus on or explicitly mention experimental design were excluded (FC3). This encompassed the use of AI for tasks within the experimental design process, such as planning, selecting, and optimizing; experiments and experimental parameters or conditions for decision-making; and the assessment of new experiments to perform next. Thus, papers that presented, for instance, the pure discovery of new materials without focusing on experiments and their parameters, were filtered out. If a different or updated version of a publication was proposed, only the newer version was included (FC4).

The filtering procedure was performed from FC1 to FC4 in an iterative manner. The papers under investigation were included until the filter criteria had been applied, after which certain publications could be excluded. The filter strategy and the filter criteria were applied to the 234 obtained publications, resulting in 22 relevant papers. In Table 1, the distribution of the excluded papers is shown in relation to the filter criteria applied.

**Table 1.** Number of studies excluded after applying each filter criterion.

| ID | Criterion | # Studies Excluded |
|---|---|---|
| FC1 | No concrete solution | 104 |
| FC2 | No AI technique | 54 |
| FC3 | Does not focus on experimental design | 55 |
| FC4 | Selection of another version | 0 |

Due to the niche of AI-driven experimental design, only a small number of contributions were included. Figure 3 presents the distribution of the 22 relevant papers by year in comparison with the 234 pre-filtered publications.

The figure illustrates the recent rise of AI in scientific research, with a particular focus on AI-driven experimental design. It is important to note that while earlier periods are grouped

into full-year ranges (e.g., 2021–2023), the most recent data cover only 2024 and the beginning of 2025 (2024–2025). As a result, the apparent decline in the number of papers in the period 2024–2025 is due to incomplete data and a shorter interval rather than to a decrease in interest in AI. However, the figure indicates growing attention to AI-driven experimental design, as even within the shorter period of 2024–2025, an emerging trend can be observed.

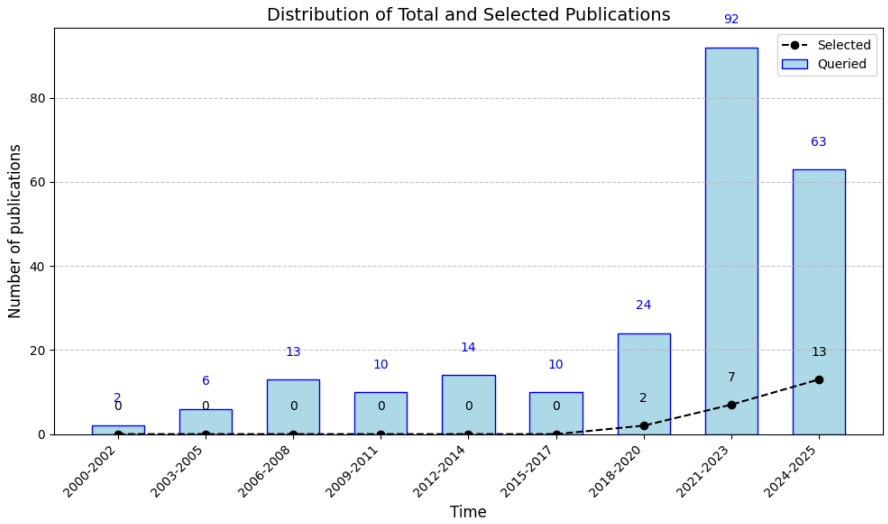


**Figure 3.** The distribution of all publications before filtering and after filtering.

### *2.3. Application of Filter Criteria*

In order to improve the comprehensibility of the filtering process, this section provides a detailed explanation of the reasons leading to the exclusion of publications based on each filter criterion. An overview of the 212 excluded publications with respect to each criterion can be found in Table 2.

**Table 2.** Overview of publications excluded based on each filter criterion.

| ID | Criterion | # Studies Excluded |
|---|---|---|
| FC1 | No concrete solution | [2–10,12–106] |
| FC2 | No AI technique | [107–160] |
| FC3 | Does not focus on experimental design | [161–215] |
| FC4 | Selection of another version | |

#### 2.3.1. Filter Criterion 1

Since the goal of this study is to discover an ideal framework for AI-driven experimental design, publications that did not propose a concrete solution by presenting or implementing a novel method, algorithm, framework, or system were excluded. This encompassed, for example, publications that only provided an overview of the literature and the corresponding state of the art, such as reviews [3–7,9,11–13,15–17,21,41,44,58,61,74,87,98,103]. As a specific example, the review proposed by Su et al. [3] discussed the current state of LLMs for catalyst design.

Furthermore, FC1 also filtered out papers that only proposed ideas and theoretical frameworks, such as perspective papers [2,8,10,19,25–27,30,33,39,40,43,46,47,49,51,65,78,79,84]. For example, a perspective paper was presented by Hysmith et al. [2] that discussed the future of self-driving laboratories.

#### 2.3.2. Filter Criterion 2

This research focuses on AI-driven experimental design. Consequently, frameworks that did not leverage AI or machine learning techniques, such as rule-based

systems (e.g., hard-coded decision rules or hand-crafted expert systems without learning or adaptation) or classical optimization algorithms without learning capabilities (e.g., grid search, brute-force search, or exhaustive enumeration) were excluded from this study. Only frameworks that incorporated models capable of learning from data were considered. Thus, publications that did not leverage AI methodologies, such as [107,108,111,117,120,124–126,131,133,136–139,142,153], were excluded. For example, Wang et al. [125] presented an approach for promoting molecules selectively to chemically active energy levels, without applying AI methodologies. In addition, papers that did not explain the underlying methodology in detail, such as Guevarra et al. [116], were excluded.

#### 2.3.3. Filter Criterion 3

FC3 was used to exclude publications that presented a concrete solution based on AI methodologies but did not target experimental design, such as [161–171]. For example, a framework was proposed by Amuzuga et al. [171] that used AI methodologies, but instead of focusing on experimental design, AI was used for metamodeling to estimate the fatigue life of a welded joint.

In addition, publications that exclusively focused on the discovery of materials, such as [193,216], or drug combinations, such as [182], in terms of only predicting appropriate output combinations without including the experimental parameters, were excluded.

#### 2.3.4. Filter Criterion 4

As a result of filter criteria FC1-FC3, there were no remaining publications that existed in different versions, leading to zero exclusions due to FC4.

### *2.4. Taxonomy*

This study aims to review the current state of research in AI-driven experimental design. To achieve this, the selected studies were carefully analyzed, based on the following taxonomy. By applying this taxonomy to the relevant contributions, the defined research questions could be addressed. Consequently, six taxonomy categories were chosen: domain of application, AI methodologies for experimental design, degree of automation, kind of data, online-capable, and generalization capability.

On a surface level, the contributions were examined by highlighting the fields and domains in which machine learning techniques or AI have been applied for experimental design. Therefore, a distinction between generic and subject-oriented frameworks could be made. Thus, the main fields of interest for AI-driven experimental design were determined.

By delving deeper, the contributions were investigated regarding the AI methodology used. Since the goal of this research is to provide a comprehensive overview of AI-driven experimental design, a key focus is to analyze the specific tasks within the experimental design process for which these AI methodologies were applied. Furthermore, the degree of automation of the reviewed frameworks was analyzed by classifying them into three categories: fully autonomous, partially autonomous, and supportive. In addition, the kind of data was investigated to identify those typically utilized in experimental design applications. Moreover, online-capable and generalizable frameworks were identified. While the former is necessary for adapting experiments on the fly, the latter offers the possibility to use a framework in different experimental design applications.

## 3. Results

This section discusses the results obtained from analyzing the pool of 22 relevant studies after carefully applying the previously defined taxonomy. A list of studies with respect to the key points investigated is provided in Tables 3 and 4.

**Table 3.** Overview of the analyzed papers regarding domains, applications, techniques, and tasks.

| Authors | Domain | Application | Technique | Task |
|---|---|---|---|---|
| Aldeghi et al. [217] | General framework | Chemistry | Tree-based regression | Assistance in robustness estimation |
| Hickman et al. [218] | General framework | Chemistry | BO | Optimization of experimental constraints |
| Schilter et al. [219] | Chemistry | Optimization of different terminal alkynes' reaction routes | BO | Selecting experiments and optimizing experimental design |
| Sadeghi et al. [11] | Materials science | Nano-manufacturing of lead-free metal halide perovskite nanocrystals | BO | Selecting experiments and optimizing experimental design |
| Epps et al. [220] | Materials science | Microfluidic material synthesis | Single-period RL + surrogate model (Naive classifier + GPR) | Surrogate model determines the feasibility of experimental parameters and predicts output; RL selects experiments |
| Plommer et al. [221] | Biology | Extraction of cannabinoids | RF | Prediction of experimental yields under different experiment conditions; assistance in decision-making |
| Eyke et al. [222] | Chemistry | Reduction of reaction screening | AL: ENN; single-trained models with MC dropout masks | Selecting experiments and optimizing experimental design |
| Adams et al. [216] | Materials science | Composition-structure phase mapping | BO | Selecting experiments and optimizing experimental design assisted by humans |
| Waelder et al. [223] | Materials science | Carbon nanotube growth | AL: Jump regression surrogate | Selecting experiments and optimizing experimental design |
| Yoon et al. [224] | Materials science | High-throughput electrical conductivity optimization and discovery of doped conjugated polymers | RF classifier + LASSO regression | Classifier excludes low conductivity material; regressor predicts experimental output |
| Fu et al. [225] | Fabrication | Quality control for probe precision forming in semiconductor manufacturing | GA (fitness function: PLSR) | Selecting experiments and optimizing experimental design |
| Lai et al. [226] | Materials science | Catalyst design and optimization | LLM + BO | LLM extracts process data; BO selects experiments and optimizes experimental design |
| Yonge et al. [227] | Chemistry | Temporal analysis of products | Model-based design of experiments | Selecting experiments and optimizing experimental design |
| Almeida et al. [228] | Chemistry | Sustainable chemistry processes | MOBO, AL: RF | Selecting experiments and optimizing experimental design |

**Table 3.** *Cont.*

| Authors | Domain | Application | Technique | Task |
|---|---|---|---|---|
| Almeida et al. [229] | Chemistry | Reaction optimization using kinetic modeling | AL: RF | Selecting experiments and optimizing experimental design |
| Bosten et al. [230] | Chemistry | Liquid chromatography | Assisted AL | Selecting experiments and optimizing experimental design |
| Liang et al. [231] | Materials science | Synthesis optimization for formulation of enzymes/ZIFs (zeolitic imidazolate framework) | BO | Selecting experiments and optimizing experimental design |
| Cruse et al. [232] | Materials science | Formation of impurity phases in BiFeO3 thin-film synthesis | DT classifier | Prediction of experimental output based on various conditions |
| Dama et al. [233] | Biology | Microbial metabolism mapping | Multi-period RL | Selecting experiments and optimizing experimental design |
| Suvarna et al. [234] | Chemistry | High-performance catalyst development for higher alcohol synthesis | MOBO | Selecting experiments and optimizing experimental design |
| Chen et al. [235] | Biology | Guidance of high-throughput screening | AL: Matrix completion | Selecting experiments and optimizing experimental design |
| Orouji et al. [31] | Chemistry | Optimization of transition metal-based homogeneous catalytic reactions | MOBO + EDNN (Ground-truth simulator for evaluation) | Selecting experiments and optimizing experimental design using MOBO, with evaluation by EDNN |

**Table 4.** Overview of the analyzed papers regarding automation, data, online capability, and generalizability.

| Authors | Automation | Data | Online-Capable | Generalizable |
|---|---|---|---|---|
| Aldeghi et al. [217]. | Supportive | Reaction data | Yes | Yes |
| Hickman et al. [218] | Partially autonomous | Reaction data | Yes | Yes |
| Schilter et al. [219] | Fully autonomous | Reaction data | Yes | Limited to different reactions |
| Sadeghi et al. [11] | Fully autonomous | Synthesis data | Yes | Limited due to fluidics lab platform |
| Epps et al. [220] | Fully autonomous | Synthesis data | Yes | Limited to flow chemistry |
| Plommer et al. [221] | Supportive | Extraction data and condition data | No | Yes |
| Eyke et al. [222] | Partially autonomous | Reaction data | Yes | Yes |
| Adams et al. [216] | Partially autonomous | X-ray diffraction data | Yes | Limited to domain experts |
| Waelder et al. [223] | Fully autonomous | Catalyst reaction data and Raman spectrum | Yes | Limited to catalyst research |
| Yoon et al. [224] | Supportive | Optical spectra and process data | No | Yes |
| Fu et al. [225] | Partially autonomous | Quality and process data | Yes | Yes |

**Table 4.** *Cont.*

| Authors | Automation | Data | Online-Capable | Generalizable |
|---|---|---|---|---|
| Lai et al. [226] | Partially autonomous | Text data and catalyst synthesis data | Yes | Yes |
| Yonge et al. [227] | Partially autonomous | Kinetic process data | Yes | Yes |
| Almeida et al. [228] | Partially autonomous | Reaction data | Yes | Yes |
| Almeida et al. [229] | Partially autonomous | Reaction data | Yes | Yes |
| Bosten et al. [230] | Partially autonomous | Chromatography data | Yes | Yes |
| Liang et al. [231] | Partially autonomous | Synthesis data | Yes | Yes |
| Cruse et al. [232] | Supportive | Synthesis data | No | Yes |
| Dama et al. [233] | Fully autonomous | Growth data | Yes | Yes |
| Suvarna et al. [234] | Partially autonomous | Reaction data | Yes | Yes |
| Chen et al. [235] | Partially autonomous | Condition data | Yes | Yes |
| Orouji et al. [31] | Partially autonomous | Catalyst reaction data | Yes | Limited to catalyst research |

The following sections focus on specific aspects found in the tables.

### 3.1. Domains of Application

AI-driven experimental design has been used in several domains to accelerate experiments, although general frameworks have also been proposed. In order to make the research comprehensible, the relevant contributions were classified into five classes based on the domains of the included contributions: general frameworks, biology, chemistry, materials science, and fabrication. The distribution of the defined domains in which AI-driven experimental design has been applied can be found in Table 5.

**Table 5.** Number of papers per domain.

| Domain | Amount |
|---|---|
| General frameworks | 1 |
| Biology | 3 |
| Chemistry | 9 |
| Materials science | 8 |
| Fabrication | 1 |

The table shows that AI-driven experimental design has mostly been applied in chemistry and materials science. This may be because these domains typically involve a large number of experiments with high-dimensional parameter spaces. In terms of chemistry, the main interest lies in reaction optimization and chemical synthesis. In materials science, AI methodologies have mostly been used in the context of materials synthesis and opti-

mization. Although a medicine-specific database was included in this research, there were no reviewed frameworks that passed the exclusion criteria.

### 3.2. AI Methodologies for Experimental Design

This section examines the machine learning and AI methodologies employed in the reviewed literature for experimental design, offering an overview of their implementations. For this study, the methodologies are grouped into four categories: optimization, supervised learning, active learning (AL), and reinforcement learning (RL). A sketch of these methodologies can be found in Figure 4.

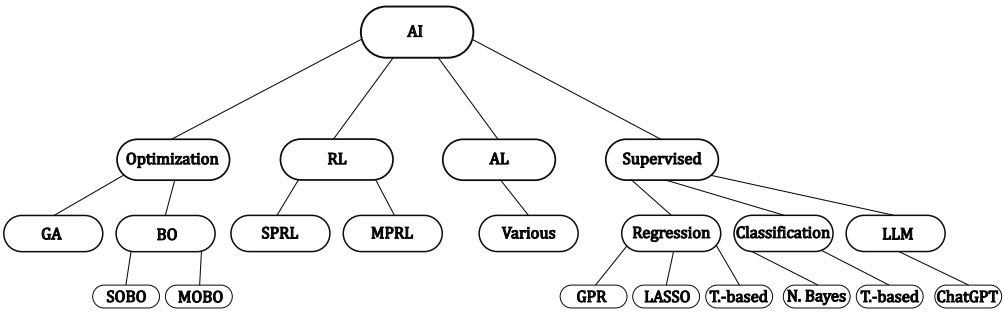


**Figure 4.** An overview of the different AI classes, methodologies, and techniques used in this survey.

These categories were defined based on their primary functional objectives. Optimization refers to algorithms whose core purpose is to iteratively improve a target outcome but may not necessarily be efficient, such as Bayesian optimization (BO) and genetic algorithms (GAs). Supervised learning refers to models trained on labeled datasets to predict or classify outcomes, such as regression and classification models. AL incorporates methods that use models to select data points (experiments) that are most informative for improving the model. It aims to enhance the learning process by reducing the amount of data required for effective model training. RL encompasses methods in which agents learn optimal actions through interaction with an environment using reward signals.

While there is an acknowledged conceptual overlap among these categories, particularly between optimization and active learning, this study adopted a function-oriented classification and did not aim to clearly distinguish the different classes using explicit definitions. Table 6 shows the number of AI techniques found in the reviewed literature under each category. The numbers in parentheses represent techniques used independently without being combined with other techniques.

**Table 6.** Categorical breakdown of applied AI methodologies with their frequency of occurrence. Methodologies that are part of another methodology, such as regression surrogates in BO, are not considered separately. The numbers in parentheses stand for the number of methodologies used independently, without being combined with another methodology.

| Category | Total Number (Separate) |
|---|---|
| Optimization | 10 (9) |
| Supervised | 8 (3) |
| AL | 5 (5) |
| RL | 2 (1) |

It can be observed that optimization and AL methodologies were used most frequently, especially as standalone approaches. In contrast, supervised techniques were combined with other methodologies for experimental design. By delving deeper into the methodologies to identify the utilized techniques, we have obtained the results shown in Table 7.

The table shows that the most widely applied technique was BO, followed by regression and classification methods. Various AL methodologies were employed, among them machine learning and non-machine learning techniques, but each technique only occurred once.

The implementation of the identified techniques is highlighted in the following by example frameworks. A distinction between single and hybrid approaches is made.

**Table 7.** Overview of methodologies used. Methodologies that are part of another methodology, such as regression surrogates in BO, are not considered separately.

| Methodology | Number |
|---|---|
| BO | 9 |
| GA | 1 |
| GP regression | 1 |
| Tree-based regression | 2 |
| Tree-based classifier | 2 |
| Naive Bayes Classifier | 1 |
| LLM | 1 |
| LASSO regression | 1 |
| AL | 5 |
| RL | 2 |

#### 3.2.1. Single Approaches

Based on the above-mentioned AI methodologies, various frameworks were found that incorporated a single technique. This section discusses some example frameworks, categorized by AI classes.

Optimization:

Several frameworks found in the contributions were based on BO for optimizing experiments or process parameters and selecting new experiments accordingly in an iterative manner; the implementations were mostly similar. For example, an approach for single-objective BO was proposed by Sadeghi et al. [11]. Here, an ensemble neural network (ENN) surrogate model was used for predicting the in-flow synthesis of Cu-based, lead-based metal halide perovskite nanocrystals. As a decision policy and acquisition function, expected improvement (EI) was proposed by the authors. In contrast, Suvarna et al. applied a combination of EI and predictive variance (PV) as an acquisition function to develop high-performance catalysts for higher alcohol synthesis, using a Gaussian process (GP) surrogate model.

Regarding GAs, the framework presented by Fu et al. [225] uses partial least squares regression (PLSR) and a GA for quality control in semiconductor manufacturing. The PLSR is applied to predict the experimental results and, thus, serves as a fitness function for the GA.

Supervised Learning:

Plommer et al. [221] proposed a supervised-based framework employing a random forest (RF) to predict the experimental or process output, aiming to optimize the extraction process of cannabinoids and predict the yields and extraction outcomes under different conditions. Thus, the selection of optimal process conditions and the exploration of unseen extraction yields could be achieved.

The general framework "Golem" developed by Aldeghi et al. [217] utilizes a tree-based regression model as a surrogate model to estimate robustness against variability in experimental conditions, such as noise or changing laboratories. In combination with optimization methods such as BO or GA, it supports the optimization of conditions and the selection of robust experiments to achieve reproducible results.

Another supervised learning approach presented by Cruse et al. [232] employs decision tree (DT) models to predict the experimental output of several synthesis conditions in terms of the formation of impurity phases in BiFeO3 thin-film synthesis.

Active Learning:

Various approaches have applied AL techniques to experimental processes. The experimental results of the obtained data are fed back to train the models, improving and optimizing the yield of the experimental output.

Eyke et al. [222] proposed a framework for predicting the reaction yield and for selecting experiments and reactions, which are the most uncertain for the predictive model, for the reduction of reaction screening. A single-trained model with applied Monte Carlo (MC) dropout masks and an ENN is used to estimate uncertainty. The ENN performed slightly better, depending on the specific task.

Similarly, Almeida et al. [229] presented an AL framework for reaction optimization, which predicts the reaction yield and estimates uncertainty, but it is based on RF regression. The AL methodologies were utilized to optimize reactions and concrete in a case study for optimizing a Pd-catalyzed C–H arylation reaction. To select experiments to perform, an exploration–exploitation strategy is employed based on prediction and uncertainty estimation. For the first three iterations, an exploration algorithm is used, while the subsequent iterations follow an exploitation algorithm based on selecting reactions with the lowest variance obtained among the top five reactions regarding the yield.

A different approach proposed by Waelder et al. [223] regarding carbon nanotube growth uses a surrogate jump regression model-based methodology for predicting the reaction yield and estimating uncertainty. The selection of experiments is performed on the basis of an exploration and exploitation strategy. While Latin hypercube sampling (LHS) is employed for the exploration phase, the maximum yield is used for the exploitation phase.

Chen et al. [235] presented a framework for selecting experiments in the case of high-throughput screening based on margin sampling. A categorical matrix completion algorithm is utilized to estimate uncertainty.

Both [216] and Bosten et al. [230] proposed assisted AL frameworks. The former approach applies BO for selecting experiments in an iterative manner with regard to composition–structure phase mapping. Thereby, humans can add informative input to guide and further optimize the algorithm. The latter uses a retention model to predict the yield and estimate the associated uncertainty for experimental results in the case of liquid chromatography. Subsequent experiments are selected iteratively, prioritizing those expected to maximize information gain or reduce the model's uncertainty. The assisted part encompasses the integration and guidance of external sources to achieve an efficient learning process and support the proper selection of experiments, especially in the initial phase of experimentation. Herein, prior knowledge and experimental data are integrated into the retention model through Bayesian statistics.

Reinforcement Learning:

Dama et al. [233] presented an RL framework called "BacterAI" for investigating combinations of amino acids that support the growth of different bacteria. BacterAI works without prior knowledge and is therefore perfectly suitable for transfer learning. The approach consists of two agents. One incorporates a neural network (NN) surrogate model for predicting the experimental output and the fitness of the chosen condition parameter. An MC search policy-based rollout algorithm is used for the trade-off between exploitation and exploration. The other agent consists of a GA that aims to find human-interpretable rules for the obtained experimental results from the NN-based agent.

#### 3.2.2. Hybrid Approaches

Optimization and Supervised Learning:

In their work, Lai et al. [226] presented a framework for catalyst design and optimization. The authors employed an LLM equipped with a multi-objective Bayesian optimization

(MOBO) approach. The LLM serves as an experimental design preparation stage and is used to identify processes and their relevant parameters in the provided raw texts. The texts are automatically filtered from the scientific literature by a keyword-based search. The LLM applied is a ChatGPT model. BO is then utilized to optimize the surrogate model and the experimental parameters and select new experiments to perform, based on the acquisition function. A GP regression model is used as the surrogate model, while EHI is applied as the acquisition function. To enhance the learning process at the beginning of the optimization, experiments are initially selected by LHS.

Supervised Learning and Supervised Learning:

Yoon et al. [224] proposed an approach for electrical conductivity optimization and discovery of doped conjugated polymers based on two supervised learning methods. It consists of an RF classifier to filter out materials with low conductivity and a least absolute shrinkage and selection operator (LASSO) regression model, which determines the conductivity and the experimental results, respectively, using different descriptors as input, such as spectral, process, material, and measurement descriptors.

Reinforcement Learning and Supervised Learning:

Epps et al. [220] proposed a framework for accelerating microfluidic material synthesis, consisting of RL and supervised learning. The framework combines a single-period horizon strategy with a surrogate model. The surrogate model includes, among others, a naive Bayes classifier to determine the feasibility of the experimental parameters and a GP regression-based model to predict the output. The RL approach consists of a belief model, an objective function, and a decision policy. An ENN is used as the belief model and trained to predict three output parameters based on the output of the surrogate model. The objective function uses a multi-objective strategy based on the weighted mean-utility or probability sampling to turn the prediction into a single quality value. This quality value is used to adjust the decision policy based on EI and, thus, new experiments are selected. The obtained experimental results are used to further improve the models.

#### 3.2.3. Summary

This section summarizes the findings of the analysis regarding the applied techniques. In Table 8, an overview of the employed techniques and the corresponding experimental design tasks is provided.

**Table 8.** Overview of techniques used for AI-driven experimental design.

| Category | Methodology/ Technique | | Task |
|---|---|---|---|
| Optimization | SOBO | Surrogate models:<br>• GP regression<br>• ENN<br>• RF<br>Acquisition functions:<br>• EI<br>• PV | Models data using surrogate models and iteratively selects experiments based on surrogate models using acquisition functions; the obtained data are used to optimize the surrogate. |
| | MOBO | Surrogate models:<br>• GP regression<br>• ENN<br>• RF<br>Acquisition function:<br>• EHI | Optimizes multiple targets, models data with surrogate models, and iteratively selects experiments based on surrogate models using acquisition functions; the obtained data are used to optimize the surrogate. |

**Table 8.** *Cont.*

| Category | Methodology/ Technique | | Task |
|---|---|---|---|
| Optimization | GA | Fitness function:<br>• PLSR | Determines the "fitness" of parameter combinations and iteratively selects experiments based on the fitness function; biology-inspired optimization using the obtained data. It is used as an additional agent for finding a human-interpretable rule for experimental observations in an RL-based hybrid framework. |
| Supervised | LLMs | ChatGPT | Extracts data from the literature. |
| | Regression | • DT<br>• RF<br>• NN<br>• LASSO regression<br>• PLSR<br>• Jump regression<br>• GP regression | Acts as a surrogate model or fitness function; in some frameworks, DTs, RFs, and LASSO regression are used independently to predict experimental output to assist in scientists' decision-making. |
| | Classification | • RF classifier<br>• Naive Bayes classifier<br>• GP classifier | Exclusion of parameter combinations with potentially poor experimental output; GP classifier for integrating human feedback into models. |
| Active Learning | Various | Reducing uncertainty:<br>• Based on Bayesian statistics<br>• Categorical matrix completion<br>Margin sampling:<br>• ENNs<br>• Single model with applied MC dropout masks<br>Acquisition function:<br>• Combination of mean square prediction error and LHS | Iteratively selects the most informative experiments while reducing uncertainty and adapts predictive models for experimental output using the obtained data. |
| Reinforcement Learning | Single-period RL | Belief models:<br>• ENNs,<br>• GP regression<br>Objective function:<br>• Weighted mean-utility function or probability sampling<br>Decision policy:<br>• EI | Selects and optimizes parameters and experiments. |
| | Multi-period RL | Belief model:<br>• NN<br>Decision policy:<br>• MC search (rollout algorithm) | Selects and optimizes parameters and experiments. |

Optimization Techniques:

The optimization techniques used in the contributions encompass BO and GAs.

BO optimizes the given experimental parameters using an appropriate surrogate model and selects or suggests new experiments to perform based on a policy applied through an acquisition function. Kernel-based GP regression, ENNs, and RFs are used as surrogate models. Both single- and multi-objective BO can be found in the contributions. The former uses the EI and PV as an acquisition function, while the latter utilizes the

Expected Hypervolume Improvement (EHI) to find the optimal Pareto front. Popular BO-based algorithms include Phoenics and Gryffin [75].

Another widely employed optimization method is the GA. It is used to optimize process parameters using a fitness function to determine which parameter combination is most suitable and should be used for the next experiment by mimicking an evolutionary process related to Darwin, optimizing the derivation of rules to select experiments.

Supervised Techniques:

Supervised methods are divided into regression and classification. Regarding regression, several techniques are used for different tasks within the experimental design process. An overview of these techniques can be found in Table 8.

RF classification and naive Bayes classification are applied as classification techniques to support the preparation of experiments by determining feasibility and filtering out poor parameter combinations. GP classification is used for uncertainty estimation in an AL framework. Regression techniques are predominantly applied as surrogate models to understand the experimental data and to support the optimization of experimental parameters.

Active Learning Techniques:

AL is used within the experimental design process to select new informative experiments to perform by reducing the model's uncertainty. Thus, it supports the training of predictive models, which are, for instance, used to forecast the results of an experiment. Various strategies are used, such as uncertainty-based sampling.

Reinforcement Learning Techniques:

RL is employed in AI-driven experimental design for choosing and optimizing appropriate experimental parameters, as well as selecting experiments accordingly. The proposed strategies encompass single-period and multi-period horizon RL. The most notable approaches include belief models and decision policies based on MC search and EI.

The distribution of AI methodologies regarding the different categories can be found in Figure 5, which shows that the majority of frameworks incorporate a single AI method and that there is a predominance of optimization and AL in AI-driven experimental design. Bayesian optimization stands out as the most applied methodology.

The reviewed literature does not include methodologies that integrate deep learning into experimental design in terms of experimental selection and optimization. This could be due to the simultaneous challenges of limited data availability and the complexity of the parameter space.

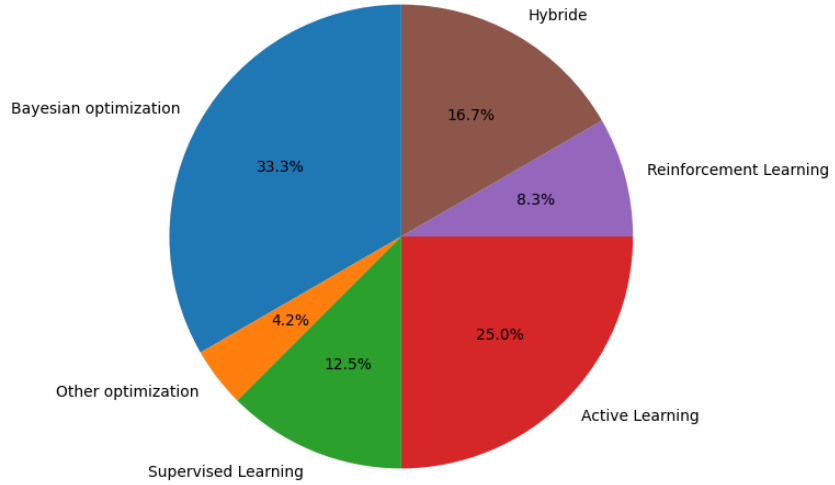


**Figure 5.** The distribution of categories (single and hybrid) across the reviewed frameworks.

### 3.3. Degree of Automation

In this section, the degree of automation of the proposed frameworks is investigated. The contributions are categorized into three classes: supportive, partially autonomous, and fully autonomous.

Within the scope of this work, a fully autonomous framework is defined as one that independently plans, selects, executes, and analyzes experiments while autonomously integrating experimental outcomes to iteratively improve its strategies. Such systems operate without any requirement for human intervention, achieving an entirely closed-loop experimental design process.

In contrast, partially autonomous frameworks perform multiple steps in the fully autonomous workflow and incorporate feedback from previous experiments. However, these frameworks do not include an automated execution and analysis stage. Partially autonomous frameworks still depend on humans to execute experiments and make decisions at critical stages, such as approving experimental suggestions or interpreting results. In the literature, these frameworks are termed "human-in-the-loop" systems, in which automation supports but does not fully replace human expertise.

Supportive frameworks provide assistance by proposing experimental candidates, narrowing the search space, or optimizing specific aspects of the experimental process. They do not autonomously adjust their strategies based on experimental outcomes and lack an iterative feedback mechanism. The final decision-making and execution processes remain entirely under human control. The classified contributions can be found in Table 4 and Figure 6, while the number of papers per automation category can be found in Table 9.

**Table 9.** The number of papers per automation category.

| Automation | Number |
|---|---|
| Fully autonomous | 5 |
| Partially autonomous | 13 |
| Supportive | 4 |

The figure shows that partially autonomous frameworks are predominantly employed. Fully autonomous and supportive frameworks are underrepresented.

Without an iterative optimization process and an autonomous experimentation platform, the objective of supportive frameworks is to model existing experimental data and predict results, making processes more efficient. Here, supervised learning techniques are employed. Using the results of experiments to optimize the models would make these frameworks partially autonomous.

Partially autonomous frameworks typically utilize AL or optimization techniques due to their iterative optimization processes. By combining an autonomous experimentation platform with a partially autonomous framework, a fully autonomous framework can be achieved.

Fully autonomous frameworks are achieved in the context of SDLs Sadeghi et al. [11], Schilter et al. [219], Epps et al. [220]. BO, AL, and RL/supervised learning are applied as AI techniques. The techniques are combined with an autonomous experimentation platform for executing and analyzing experiments. Sadeghi et al. [11] utilized a self-developed modular platform, consisting of fluid delivery, mixing and reaction, and in situ characterization. Schilter et al. [219] applied IBM's RoboRXN platform and used robotic actions by RoboRXN for executing experiments and HLPC for analyzing experimental results. Epps et al. [220] also employed a self-developed modular platform, incorporating an autonomous LHP QD synthesis bot. In the context of carbon nanotube growth, an aged-

walled, supported catalyst chemical vapor deposition system was used by Waelder et al. The system was integrated into the ARES (Automated Research System) platform.

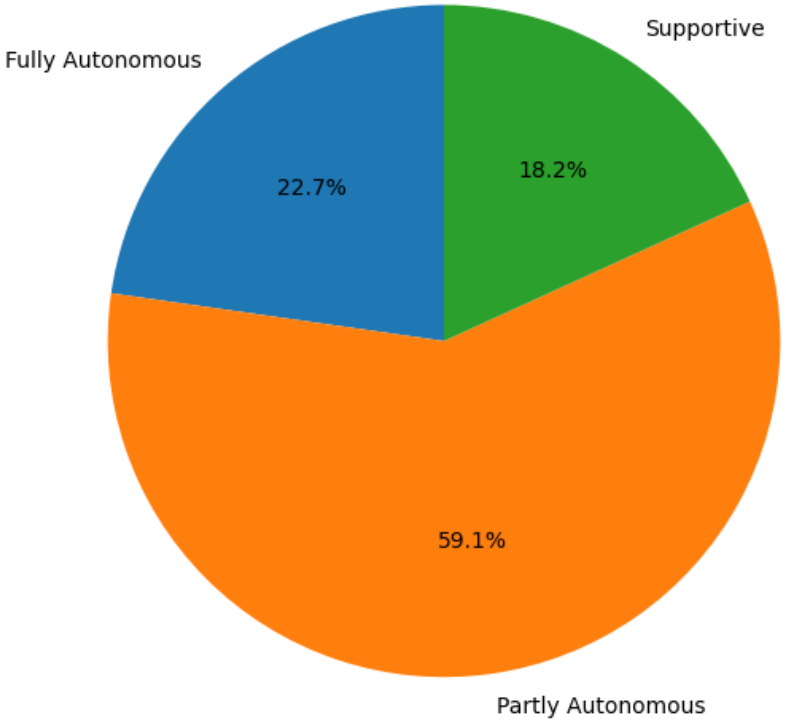


**Figure 6.** The distribution of the frameworks with regard to the degree of automation.

### *3.4. Kind of Data*

In the reviewed literature, various types of data can be found, depending on the domain and the objectives of the applied framework. Most datasets include experimental parameters specific to the field of application, such as reaction parameters, synthesis parameters, or other process-related variables, along with their corresponding experimental output. For synthesis processes, these parameters include the temperature and solvent type. In the context of microbial metabolism mapping, parameters such as growth data on amino acids or other nutrients are utilized. Additionally, some frameworks incorporate text data extracted from published scientific articles, which contain process parameters. In Table 4, the types of data and the corresponding studies can be found.

### *3.5. Online Capability*

Online-capable frameworks are important for understanding processes and experiments and adapting them on the fly. In this research, online capability refers to the incorporation of a feedback loop, in which models are updated with experimental data as soon as the results are obtained, allowing for continuous experimentation and optimization until a predefined stopping point is reached. In Table 4, the results obtained from the online capability analysis are shown, while Table 10 shows the number of papers found to be online-capable.

**Table 10.** The number of papers with regard to online capability.

| Online Capable | Number |
|---|---|
| Yes | 19 |
| No | 3 |

The results indicate that nearly all frameworks are online-capable, except for three supportive frameworks. Both of these frameworks show a lack of adjustment through the data received from selected and conducted experiments.

### 3.6. Generalization Ability

The aspect of generalizability plays an important role in deploying robust frameworks across different scenarios and applications, especially in the context of autonomous laboratories, which are ideally designed to be adaptable to diverse use cases.

In this context, "generalizability" refers to the ability of a framework to maintain its performance and reliability when applied beyond its original training domain or initial application area, without requiring significant modifications. A highly generalizable framework can be transferred to new experimental applications, materials, or objectives while still providing effective and trustworthy results. Table 4 shows the list of contributions and their generalization capability. Table 11 shows the number of generalizable papers.

**Table 11.** The number of papers with regard to generalizability.

| Generalizability | Number |
|---|---|
| Yes | 16 |
| Limited | 6 |

Some of the frameworks are limited to specific applications or materials due to the incorporation of domain-specific experimentation platforms. Other frameworks are optimized for a specific application and need to be adapted. General frameworks require domain-specific data and possibly expert knowledge and can be deployed across different scenarios and applications.

### 3.7. Discussion

While our systematic search initially identified 234 publications, the final set included only 22 papers (approximately 9%). This relatively small number is primarily due to the niche nature of the research field, as our inclusion criteria were intentionally focused on papers that directly addressed frameworks that proposed concrete solutions based on AI-driven experimental design. Filtering for AI-based and experimental design-related publications is necessary to ensure appropriate results. Future surveys could consider broader search terms or inclusion criteria to capture a wider range of contributions. For example, the term "artificial intelligence" could be replaced or extended with the terms "deep learning", "machine learning", and "automated experimentation". However, this could also increase the number of irrelevant publications found during the experimental derivation of the search query, especially by only considering "automated experimentation", " which leads, among others, to non-AI-based experimentation frameworks. Similarly, a replacement of the included experiment-related terms with the term "experimental design" also led to poor results.

The observations made during the systematic review of the literature lead to the question of what properties an ideal system or framework for AI-driven experimental design should incorporate. Depending on the application's objective, one has to decide whether a system needs to operate partially or fully autonomously. Both frameworks are capable of using AI to plan and select experiments and optimize future experiments based on the obtained experimental results, e.g., Lai et al. [226] (partially autonomous) and Epps et al. [220] (fully autonomous). While partially autonomous frameworks can play a supporting role for scientists during the experimental design process to overcome expensive trial-and-error experiments, fully autonomous frameworks perform the selected

experiments without the need for a scientist in the loop. In contrast, supportive frameworks are not desirable due to the missing feedback loop. Thus, such systems are not able to learn from the new observations obtained during experiments. Compared to partially autonomous frameworks, fully autonomous frameworks are significantly less represented in the reviewed literature, which shows the need for further implementations in this field. However, both partially and fully autonomous frameworks share similar desired properties. Both need to be generalizable in order to be used for different applications. A majority of the reviewed frameworks exhibit generalizability. This is particularly important for fully autonomous systems, which are usually applied in the context of SDLs and, thus, should perform different kinds of experiments without being limited to one specific kind. An example of a limited framework was proposed by Epps et al. [220] that focused on flow chemistry. Therefore, the experimentation stage needs to be more flexible and adaptable. Furthermore, online capabilities are necessary to adapt experiments based on newly collected data. All partially and fully autonomous reviewed systems meet this criterion.

In terms of AI techniques, AL (including optimization) and RL should be applied. Both methodologies incorporate a feedback loop and an adaptation based on newly received data. A key limitation of existing frameworks is the sparse availability of real, domain-specific data, which is both time-consuming and costly to obtain. Particularly in the early stage, sufficient data are mandatory for an efficient exploration. While optimization techniques and AL are generally efficient in handling sparse data, RL- and supervised learning-based methodologies require large amounts of data to achieve effective learning and generalization. Particularly, AL is capable of integrating human knowledge for dealing with scarce data, enhancing learning efficiency and speed. Other general but potential solutions to overcome the data bottleneck include the use of transfer learning, few-shot learning, and data augmentation techniques [236,237]. An approach for integrating both human knowledge and generative AI to deal with scarce data is membership query synthesis. Here, generative AI is applied to generate synthetic data based on real experimental data while incorporating the knowledge of human scientists in terms of AL to enhance data quality [238].

In addition to data scarcity, the complexity of the data is often high due to the high-dimensional parameters and search spaces. Multi-objective-based optimization frameworks and reinforcement learning aim to handle this problem. Although MOBO is suitable for low-data environments, it may struggle to achieve a good trade-off between multiple objectives when data are too scarce or with insufficient computational resources. An advantage of RL over optimization methods is the planning of multi-step strategies, while optimization methods suggest one experiment at a time. Apart from this, Dama et al. [233] showed that RL is also able to learn experimental design without prior knowledge, leading to high generalizability. In conclusion, an ideal framework could integrate AL with RL, referred to as reinforcement active learning, to address both limited data availability and the complexity arising from high-dimensional parameter and search spaces.

A preferable improvement for the methodologies discussed, besides data augmentation, is DL as a state of the art methodology. It enhances the adaptation to newly received data, capturing complex patterns in high-dimensional spaces, thereby increasing predictive accuracy. However, the reviewed literature lacks a framework that incorporates DL. One reason is the previously mentioned data scarcity. DL models typically require large, labeled datasets to generalize effectively. Moreover, the computational cost and infrastructure requirements for training and deploying DL models can be prohibitive in laboratory settings that prioritize real-time decision-making and flexibility. Additionally, DL models are often treated as black boxes, which raises concerns about interpretability and explainability

when AI is expected to guide scientific decisions. In general, the explainability of AI-driven experimental design decisions remains largely unaddressed, with only one of the reviewed frameworks (Yoon et al. [224]) considering this aspect as a main research objective by incorporating a combination of an RF classifier and LASSO regression. However, some frameworks, even if not explicitly stated, deploy explainable and interpretable methodologies and are therefore considered explainable. Examples include purely tree-based frameworks (Aldeghi et al. [217], Plommer et al. [221], Cruse et al. [232]) or approaches that achieve partial explainability by integrating interpretable surrogate models, such as GP regression (Hickman et al. [218], Schilter et al. [219], Suvarna et al. [234]) or tree-based models (Liang et al. [231]). Future research should prioritize explainability to develop reliable and trustworthy frameworks and ensure acceptance among scientists.

An important aspect to consider when implementing AI-driven experimental design frameworks is their ethical dimension. In the case of fully autonomous frameworks, they offer tremendous advantages, but several critical questions arise: Who is responsible if AI designs and conducts harmful, unnecessary, or costly experiments? Does the use of fully autonomous systems assist scientists by relieving them of monotonous, time-consuming tasks, or does it risk excluding them from the creative experimentation process? Furthermore, how can the risk be mitigated that AI frameworks inherent biases from their training data? High transparency in the AI's decisions and the operational process is needed to ensure the trust of scientists. In contrast, partially autonomous and supportive frameworks can act as a helping hand, narrowing the research space and suggesting experiments while leaving the decision-making and experimentation in human hands, thereby accelerating the research but preserving creativity. Hazardous or impractical experimental designs can be disregarded by researchers, and in partially autonomous frameworks, such feedback can be used to further refine and improve AI's recommendations. If carefully designed, both frameworks could lead to high reproducibility, reducing waste and unnecessary experiments and thereby accelerating research.

## 4. Conclusions

This study investigated the role of AI in experimental design, aiming to explore whether and how AI can accelerate scientific research. A broad literature search was conducted across multiple databases, combining method-based, subject-specific, and general sources. A carefully developed search query and appropriate filtering narrowed the initial number of 234 results to 22 relevant contributions. This relatively small number of results reflects the emerging nature of AI-driven experimental design, highlighting a clear need for further research in this interdisciplinary field. A taxonomy-based analysis of the selected studies was used to address the defined research questions.

The findings suggest that AI has significant potential to accelerate scientific research by optimizing the design, planning, and execution of experiments. In particular, AL, including optimization methodologies, stand out as key drivers, enabling iterative refinement of experiments using minimal data. These methods can effectively reduce the number of necessary trials by prioritizing the most informative experiments, thus saving time and resources. The use of surrogate models and uncertainty estimation allows AI systems to make informed decisions, even under data scarcity, demonstrating a practical advantage over traditional trial-and-error methods. BO is predominantly employed and shows great performance in handling scarce data and multiple targets (MOBO). To address scarce data and high-dimensional parameter spaces and enable long-term planning, combining RL with the data efficiency of AL is recommended.

Apart from this, the majority of AI frameworks belong to chemistry or materials science. The generalizability of several frameworks offers the opportunity to apply them in other domains.

However, the application of DL remains limited, primarily due to data requirements. Obtaining significant amounts of real data is often time-consuming and costly. Therefore, future research should investigate data-efficient frameworks and AI methods for dealing with scarce data. Where sufficient data is available, its integration could lead to more powerful, flexible, and accurate design tools. Data augmentation, transfer learning, and few-shot learning could help to overcome data scarcity. Furthermore, the lack of explainability and transparency in AI decision-making remains a barrier to broader acceptance within the scientific community. This highlights the need for the implementation of interpretable models.

In terms of deployment, partially autonomous frameworks are most common, balancing AI-driven decision support with human oversight. Here, AI acts as a helping hand, without preventing human creativity. In contrast, fully autonomous systems offer transformative potential by enabling continuous, closed-loop experimentation without human intervention. These systems can drastically speed up the experimentation process by suggesting experimental designs, executing them, and analyzing the results to modify subsequent experiments. However, the implementation of fully autonomous frameworks is still rare and needs further research. In particular, regarding their explainability to address ethical issues.

Overall, this study demonstrates that AI-driven experimental design can make scientific research more efficient, targeted, and reproducible. Researchers, especially in data-rich, high-throughput environments or with high parameter-search space complexity, stand to benefit most. In addition, domains with sparse data can also see improvements through smart sampling and model-guided experimentation. This research provides a foundation for future studies that aim to apply AI for experiment design in a certain domain. By offering a structured overview of existing frameworks, their implementation, and associated limitations, this study seeks to support researchers in selecting and developing suitable AI-driven approaches to accelerate their experimental processes.

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## Abbreviations

The following abbreviations are used in this manuscript:

| | |
|---|---|
| AI | Artificial intelligence |
| AL | Active learning |
| BO | Bayesian optimization |
| DL | Deep learning |
| DT | Decision tree |
| EDNN | Ensemble deep neural network |
| EHI | Expected hypercube improvement |
| EI | Expected improvement |
| ENN | Ensemble neural network |
| FC | Filter criteria |
| GA | Genetic algorithm |
| GP | Gaussian process |
| LASSO | Least absolute shrinkage and selection operator |
| LHS | Latin hypercube sampling |
| LLM | Large language model |
| MC | Monte Carlo |
| MOBO | Multi-objective Bayesian optimization |
| NN | Neural network |
| PLSR | Partial least square regression |
| PV | Predictive variance |
| RL | Reinforcement learning |
| RF | Random forest |
| SOBO | Single-objective Bayesian optimization |

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