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A Conceptual Model for Improving Perovskite Solar Cells Efficiency Using Machine Learning

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Abstract

Solar cells made from perovskites have experienced rapid development as examples of third-generation solar cells in recent years. The traditional trial-and-error method is inefficient, and the search space is incredibly large. This makes developing advanced perovskite materials, as well as high conversion efficiencies and stability of perovskite solar cells (PSCs), a challenging task. A growing number of data-driven machine learning (ML) applications are being developed in the materials science field, due to the availability of large databases and increased computing power. There are many advantages associated with the use of machine learning to predict the properties of potential perovskite materials, as well as provide additional knowledge on how these materials work to fast-track their progress. Thus, the purpose of this paper is to develop a conceptual model to improve the efficiency of a perovskite solar cell using machine learning techniques in order to improve its performance. This study relies on the application of design science as a method to conduct the research as part of the study. The developed model consists of six phases: Data collection and preprocessing, feature selection and engineering, model training and evaluation, performance assessment, optimization and fine-tuning, and deployment and application. As a result of this model, there is a great deal of promise in advancing the field of perovskite solar cells as well as providing a basis for developing more efficient and cost-effective solar energy technologies in the future.

Keywords

Perovskite Solar Cell, Machine Learning, Solar Energy, Design Science Research

1. Introduction

A huge challenge is to find sustainable and clean energy sources that will meet the needs of a growing global population and industrialization, in order to meet their growing demands [1]. Photovoltaics could prove to be a viable solution to the energy crisis we are experiencing [2]. It has been proven that silicon-based solar devices and modules have been highly efficient and have achieved more than 26% efficiency for single crystal devices and 22% efficiency for multi-crystal devices [3]. Nevertheless, the energy-intensive purification process necessary for the manufacturing process has caused researchers to explore alternative forms of photovoltaic technology, including organic and perovskite-based absorbers, as alternatives to the energy-intensive purification process required in their production [4]. Cost issues are a significant challenge when it comes to the manufacture, installation, operation, and maintenance of commercial silicon photovoltaic systems. In this sense, they are now able to play a significant role in providing a substantial contribution to the global energy need. During the course of maintaining, repairing, and ultimately replacing production equipment, more fossil fuels will be needed in order to perform these activities.

The PSC market has been experiencing unprecedented success compared with the commercial silicon solar cell market [5] [6]. During the early years of the research, a large part of the effort was dedicated to improving the efficiency of the system. In 2009, the authors of [7] reported that they made the first PVs with a power conversion efficiency (PCE) of 3.8% by using organic-inorganic halide perovskites as the source of light. A great deal of progress has made sense when it comes to improving the PCE of PSCs in recent years. Moreover, over the past few years, the performance of these PSCs has improved significantly to reach over 25.5% [8]. As PSCs became increasingly efficient and stable, new issues began to arise that raised new concerns and a need for research subsequently [9]-[11]. Almost all the research that has been conducted on perovskites has focused on inorganic perovskites, hybrid organic-inorganic perovskites (HOIPs), and double perovskites from the point of view of composition and structural classification [12] [13]. For example, the organic component of HOIPs enables them to have extra functions and a certain level of structural flexibility that are not achievable in the case of pure inorganic perovskites. The different structural and chemical variations of these molecules provide ample opportunities to tune and modulate the physical properties of these molecules simply by altering their chemical composition [14]. As a result of the use of double perovskites, it opens up a new dimension of possibilities: the use of different metal cations at both the A and B sites may provide more options, leading to a higher PCE and wider bandgap [15]. In addition, inorganic perovskites are generally known to have a high degree of thermal stability [16]. Data-driven machine learning has been shown to be an effective tool in screening candidates, as well as a powerful tool for predicting candidates based on experimental validation, when compared with traditional methods [17].

Therefore, this paper aims to develop a conceptual model for improving the perovskite solar cell's efficiency using machine learning. A research methodology associated with design science refers to the kinds of research approaches that are derived from the design science paradigm in order to continue with this topic. The developed model consists of six phases: Data collection and preprocessing, feature selection and engineering, model training and evaluation, performance assessment, optimization and fine-tuning, and deployment and application.

This paper is organized as follows: the methodology is discussed in Section 2. The limitations of the study are presented in Section 3, whereas the conclusion and future works are presented in Section 4.

2. Methodology

This study used design science research [18] [19] to develop the conceptual model for improving the perovskite solar cell's efficiency using machine learning. The purpose of design science research is to identify problems and solve them through the application of design principles. Even though it is considered to be able to balance the relevance of research with the rigor of its methodology, it has become increasingly accepted and adopted by information systems researchers as a legitimate method for conducting research, because it provides a mechanism for balancing relevance with rigor in the research process. Thus, the adapted methodology is used to develop the conceptual model for improving the perovskite solar cell's efficiency using machine learning as shown in **Figure 1**. This model leverages the power of AI and machine learning algorithms to identify and optimize key parameters, leading to the improved efficiency of perovskite solar cells. The developed conceptual model for improving perovskite solar cell efficiency using machine learning consists of six phases as shown in **Figure 2**.

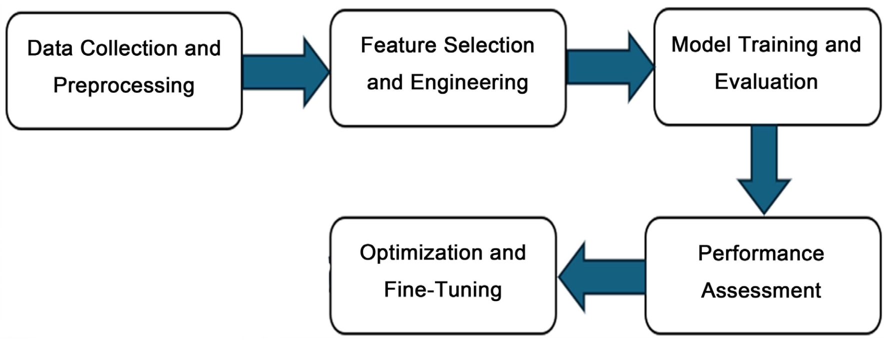

Figure 1. Conceptual model for improving the perovskite solar cell's efficiency using machine learning.

1) ***Data Collection and Preprocessing***: During the first step of creating a model, it is necessary to collect experimental data from a variety of sources so that the model can be created. It is possible to consider the composition of the perovskites, the structure of the device, operational conditions, and external environmental factors when designing a device. It is necessary to cleanse, organize, and normalize the data once it has been collected in order to ensure its consistency and usability when it comes to machine learning techniques after it has been collected. **Figure 2** displays the data collection and preprocessing phase. There are many data collected samples, including for example: the effect of temperature on the properties of perovskites, such as crystal structure, photoluminescence, and conductivity, pressure, water vapor permeability, humidity-related degradation, solar light, and artificial light on perovskites. The method used in this data preprocessing is driven by the principle of relative theory. Relative theory is a data-driven approach that focuses on identifying patterns and relationships within the data. It relies on the idea that data can be compared and analyzed relative to one another rather than solely based on absolute values.

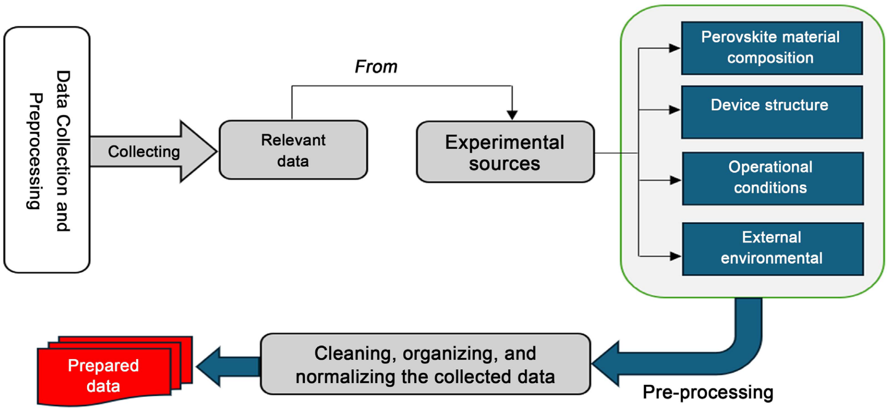

Figure 2. Data collection and preprocessing phase.

2) ***Feature Selection and Engineering***: The next step in the process is to analyze the data to identify which features in the data can accurately reflect a device's performance. Selecting features allows you to filter out irrelevant or redundant ones, whereas engineering features means you are able to make them more useful for machine learning models by improving their usefulness. By simplifying the dataset and reducing the complexity of the model, the purpose of this step is to improve the accuracy of predictions by simplifying the dataset and reducing the complexity of the model. Figure 3 illustrates the feature selection and engineering. The feature extraction equation used is Y = f(X). In this equation, the output of the model (y) depends on the learned features (f) derived from the input data (X). The learned features can be derived through various techniques such as feature extraction, feature selection, or dimensionality reduction. The goal of these techniques is to extract the relevant information from the input data that correlates with the target variable (efficiency or performance).

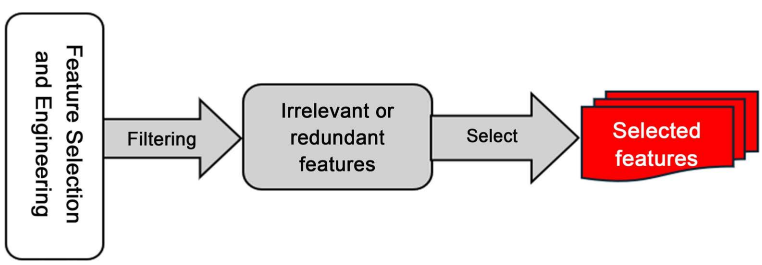

Figure 3. Feature selection and engineering phase.

3) ***Model Training and Evaluation***: The training of the model can be done by choosing features and preprocessing the data prior to using machine learning algorithms. There are several deep learning models currently available in the market, among which are convolutional neural networks (CNN), recurrent neural networks (RNNs), and ensembles. In this phase, we consider the relationships between the features of perovskites and their performance parameters to predict and optimize their performance. Figure 4 demonstrates the model training and evaluation phase.

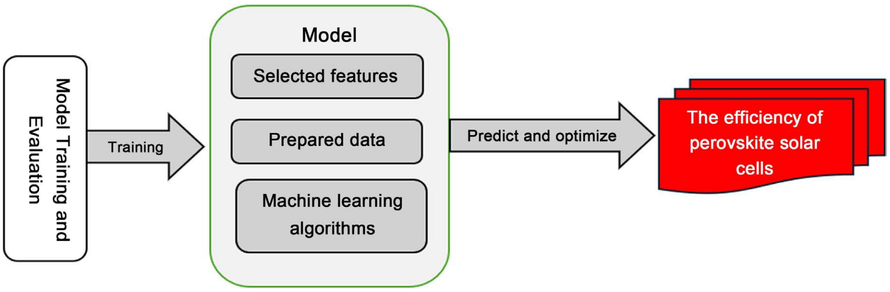

Figure 4. Feature selection and engineering phase.

4) ***Performance Assessment***: To assess the performance of the trained model, it can be applied to unseen data. This can be done by testing the model's ability to predict the efficiency values on new device structures or operating conditions. Performance metrics such as accuracy, precision, recall, and F1-score can be used to evaluate the model's effectiveness. Figure 5 displays the performance assessment phase. The calculation formulas for the evaluation parameters are:

- **Current Density (J)**: J = I/A. where J is the current density, I is the electric current, and A is the area of the sample.
- **Open Circuit Voltage (Voc)**: Voc = V − Vm. where Voc is the open-circuit voltage, V is the voltage across the cell, and Vm is the voltage of the measurement reference.
- **Short Circuit Current (Isc)**: Isc = Imax − Imin. where Isc is the short circuit current, Imax is the maximum current, and Imin is the minimum current.
- **Light-to-Electric Power Conversion Efficiency (Lppe)**: Lppe = (Pout − Ploss)/Pinc. where Lppe is the light-to-electric power conversion efficiency, Pout is the output power, Ploss is the power loss, and Pinc is the incident power.
- **Voltage Stability (Stability)**: Stability = (Vmax − Vmin)/Vmax. where Stability is the voltage stability, Vmax is the maximum voltage, and Vmin is the minimum voltage

5) ***Optimization and Fine-Tuning***: The model can be optimized and refined to improve its predictive capabilities based on the performance evaluation results. This involves adjusting model hyperparameters, such as learning rates, regularization terms, and network architectures, to optimize its performance. Fine-tuning the model helps achieve more accurate and efficient predictions, leading to

improved perovskite solar cell efficiency. Figure 6 displays the optimization and fine-Tuning phase.

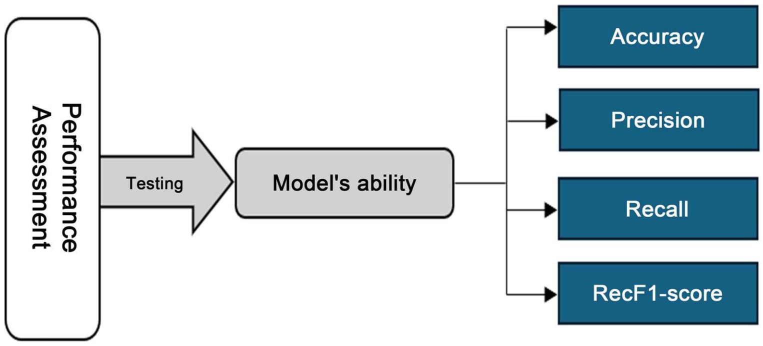

Figure 5. Performance assessment phase.

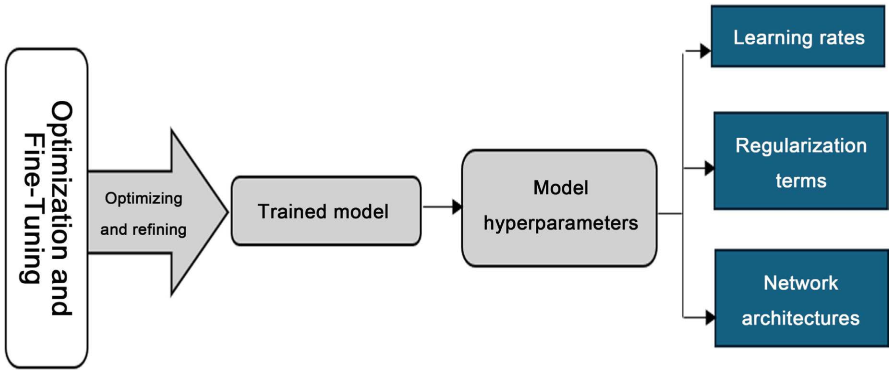

Figure 6. Optimization and fine-Tuning phase.

3. Limitations

This section discusses the limitation of the developed conceptual model for improving perovskite solar cell efficiency using machine learning. Table 1 displays the limitations of the developed model for improving perovskite solar cell efficiency.

Table 1. Limitations of the developed Conceptual model for improving perovskite solar cell efficiency using machine learning.

Limitation	Explanation
Lack of Standardization and Robust Testing	The developed model is based on a specific conceptual model, which may not apply to all perovskite solar cell devices. Due to the diversity of perovskite solar cell materials and designs, a universal model covering all scenarios may not be feasible. Therefore, the effectiveness and applicability of the developed model may be limited to the specific types of perovskite solar cells.
Data Dependency and Bias	Machine learning algorithms heavily rely on data to make predictions. However, the quality of the data can significantly impact on the model's performance. The developed model relies on training data which may contain bias or errors that affect the prediction. These biases may limit the accuracy and reliability of the results.

Continued

Complexity and Interpretability	Machine learning algorithms can be complex, making it difficult to understand the reason behind the decisions made. the developed model relies on complex models, which can make it difficult to interpret the results and justify optimization decisions. This lack of transparency may hinder the widespread adoption and trust in the approach.
Scalability and Maintenance	The developed model requires significant computational resources and time to train and validate the model. As the number of perovskite solar cell devices increases, it becomes impractical to apply the developed model to every device individually. Additionally, the model may become obsolete over time, requiring continuous updates to maintain its effectiveness.
Human Interaction and Autonomy	processes, human intervention is still necessary. Experienced experts are still required to interpret the results, select appropriate training data, and make decisions on optimization targets. Moreover, the developed model may not be suitable for all optimization tasks, as some require human intuition or experimentation.

4. Conclusion

In recent years, perovskite solar cells have experienced rapid development as examples of third-generation solar cells. As a result of the traditional trial-and-error method, the search space is extremely large and inefficient. Due to this, PSCs are challenging to design due to their high conversion efficiencies and stability. Due to large databases and increased computing power, materials science is increasingly developing data-driven ML applications. For fast-tracking the development of new perovskite materials, machine learning can be used to predict their properties and expand our understanding of how they work. Hence, this paper developed a conceptual model that uses machine learning techniques to improve perovskite solar cell efficiency. During the course of the study, design science is used as a method to conduct research. The developed model consists of six phases: data collection and preprocessing, feature selection and engineering, model training and evaluation, performance assessment, optimization and fine-tuning, and deployment and application. Through this model, perovskite solar cells will be advanced and a basis for developing more efficient and cost-effective solar technology will be provided in the future. The future work of this study is to implement the developed model in real scenarios to demonstrate the effectiveness of the developed model.

Conflicts of Interest

The author declares no conflicts of interest regarding the publication of this paper.

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