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Machine learning-driven insights into efficiency optimization of Si solar cells assisted by $CH_3NH_3PbBr_3$ perovskite and WS_2 nano-structures

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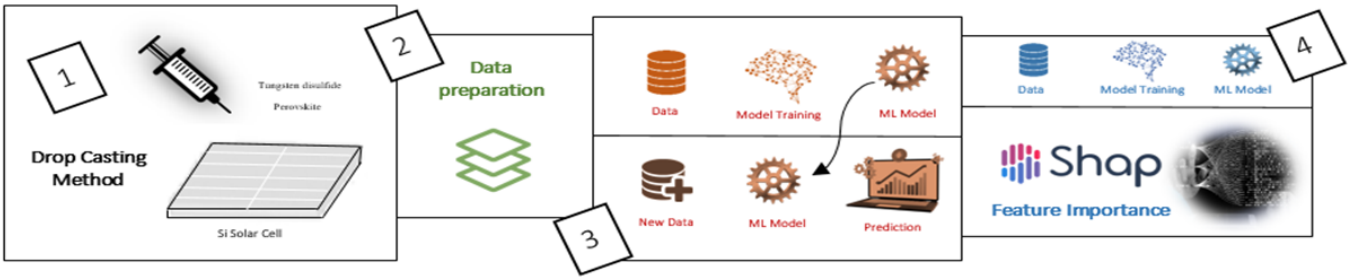
Abstract

Machine learning techniques, by leveraging advanced algorithms can pave the way for the development of more efficient solar cells by accurately predicting their efficiency and identifying the most influential features that affect their performance. Identifying the most influential features facilitates the optimization of experiments while predicting efficiency reduces the number of experiments. This approach saves time and costs and ultimately, efficient solar cells will play a useful role in solving the energy crisis as renewable energy sources. For this purpose, in the first step of this study, machine learning techniques are used to predict the relative efficiency of silicon solar cells for 58 experimental data after drop-casting with certain concentrations of tungsten disulfide and $CH_3NH_3PbBr_3$ perovskite nano-structures. It was found that the extreme gradient boosting model has the best performance. This model also showed promising results for 12 new data. In the second step, Shapley additive descriptions will investigate the most influential feature on cell efficiency. According to the SHAP results, deposition of tungsten disulfide nano-structures after perovskite on the silicon solar cell surface has the best performance to increase efficiency. In fact, the sequence of drop-casting of each kind of the nano-structures influences the efficiency based on the different interaction mechanisms.

Graphical Abstract



1. Introduction

Human activities, including burning fossil fuels, deforestation, and industrial activities, have many impacts, including rising temperatures, rising sea levels, and more frequent and intense storms. The increase in greenhouse gases in the last century has also threatened the Earth with global warming. These changes have profound consequences and are considered a danger to modern society. While the world is facing an energy shortage problem, one of the main measures to address this threat is the transition from fossil fuels to renewable energy sources. Solar energy is recognized as a suitable renewable energy source due to its versatility and abundance[1].

As a renewable energy source, solar cells pave the way for entering a carbon-free society. Over the years, many efforts have been made to improve the efficiency of the silicon solar cells. Research has shown that materials such as zinc oxide, transition metal dichalcogenides such as tungsten disulfide and molybdenum disulfide, and organic hybrid perovskites can act as suitable candidates for improving the efficiency of solar cells[2–4]. Tungsten disulfide, of the transition metal dichalcogenides (TMDCs) family, is a promising material in photovoltaic applications with band gap tunability, high absorption coefficient, and unique optical and electrical properties. WS_2, exhibits excellent optical properties, such as strong absorption in the visible and near-infrared regions. Its 2D structure supports exciton generation and enhances light trapping, reducing reflection losses[5]. On the other hand, $CH_3NH_3PbBr_3$ perovskite shows a high absorption coefficient and broad absorption spectrum, which promote the absorption of silicon. This synergy improves the overall light-harvesting capability of the solar cell[6]. Coating silicon solar cell with WS_2 and $CH_3NH_3PbBr_3$ nano-structures reduces surface recombination by passivating dangling bonds and defects on the surface. Moreover, The WS_2 and $CH_3NH_3PbBr_3$ layers form heterojunctions with silicon, and facilitate charge carrier separation. Also, the heterojunction creates an additional electric field at the interface, which enhances charge carrier mobility and extraction. Both WS_2 and perovskite coatings can act as anti-reflective layers, which allows more photons to penetrate the silicon substrate, contributing to higher photocurrent generation[7,8]. Depositing tungsten disulfide after $CH_3NH_3PbBr_3$ perovskite optimally strengthen the performance of both materials. This sequence ensures effective light absorption, charge transport, and surface passivation while improving the stability and durability of the solar cell. Consequently, this configuration achieves the highest efficiency gains in silicon solar cells.

For this purpose, in this work, the surface of silicon solar cells was deposited by different concentrations of tungsten disulfide and $CH_3NH_3PbBr_3$ perovskite suspension using the drop-casting method. The results of the current-voltage curves of the cell in the raw state and after each drop showed that the concentration of 1 g/l of tungsten disulfide with 11.46% enhancement and the concentration of 2.5 g/l of perovskite with 17.77% enhancement have the best performance. To date, the role of tungsten disulfide and organic hybrid perovskites in solar cell efficiency has been investigated using traditional laboratory techniques based on trial and error. Despite their many successes, these methods impose much time and cost. Predicting efficiency and identifying and interpreting the most influential experiment parameter on solar cell performance can lead to experiment optimization. In this regard, machine learning techniques have recently played a useful role in basic research. ML performs certain tasks by learning from data and identifying patterns. Studies have shown that the use of ML techniques can significantly accelerate research[9,10]. In this regard, the photovoltaic community has also benefited from the effectiveness of ML[11,12]. In recent years, ML algorithms have been used in various aspects of solar cells, including device manufacturing, defect classification, examining the most influential parameters, and efficiency

prediction[13–17]. Therefore, ML techniques can play an important role in solving the energy crisis by improving the performance of solar cells.

Here, we focus on the efficiency changes data of silicon solar cells when the cell surface is coated with tungsten disulfide and perovskite nano-structures. Given this field's limited number of experiments, choosing a suitable machine-learning model is the main challenge. Random forest, gradient boosting, and XGBoost algorithms adapt well to small datasets. Therefore, in this study, the first step investigates ML's ability to predict the relative efficiency of solar cells using these algorithms, and the second step investigates the effect of the presence of the second nanomaterial on the changes in cell efficiency using SHAP values.

2. Method

As shown in Fig. 1, after coating silicon solar cells with different concentrations of tungsten sulfide and perovskite, the solar cell performance parameters were calculated directly from the measured current and voltage data using a Python function. Then, the relative cell efficiency, which is the cell efficiency per drop of WS_2 and perovskite concentration relative to the cell efficiency before coating, was taken as the target. In the next steps, machine learning techniques were used to predict cell efficiency and identify the most influential feature on cell efficiency.

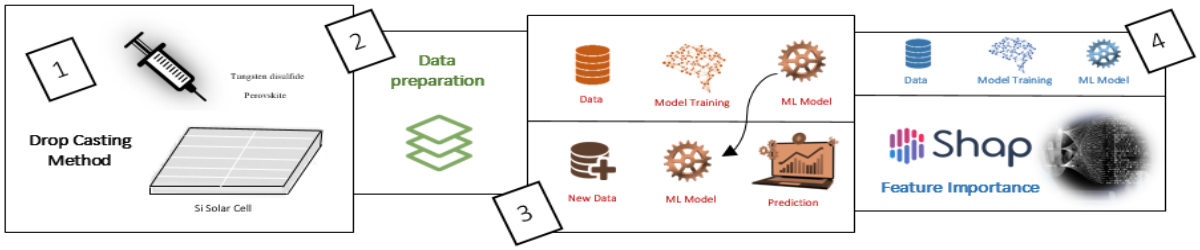


Fig 1. Step-by-step process of the study methodology.

2.1. Prediction Model

In the first step, ML techniques are used to predict the relative efficiency of the cell. For this purpose, a dataset containing 58 Rows including two categorical features to describe the presence or absence of the second nanomaterial and the order of use of nanomaterials and 4 numerical features including the concentration value and the number of tungsten disulfide and perovskite droplets was created. 80% of the data set was considered the training set and the remaining 20% was the test set. The two categorical features were converted to numerical values by ordinal encoding, where 0 means no material, 1 indicates perovskite, and 2 indicates tungsten disulfide. It should be noted that these numerical values do not indicate a specific order and were used only as identifiers.

The ML prediction model was built using random forest, gradient boosting, and extreme gradient boosting algorithms. These algorithms are suitable for working with small datasets[18]. The ML models were evaluated based on coefficient of determination and root mean square error metrics. Bayesian optimization was also used for hyperparameter tuning. This method performs better than random or grid search by creating a probabilistic model of the objective function and considering previous evaluations.

2.2. Feature Importance Analysis

In the second step, to investigate the effect of the presence of the second nanomaterial on cell efficiency, the amount of perovskite and tungsten disulfide in each drop of different concentrations was calculated. In this calculation, each drop was considered equal to 0.05 cc. In this way, the numerical features of the data set were reduced to two columns of nanomaterial amounts. Sorting the data set in this way simplifies the data structure and makes it easier to interpret the most influential feature on the relative efficiency of the cell. Also, the Variance Inflation Factor (VIF) results in Table 1 indicate the absence of significant multicollinearity. This leads to a more accurate interpretation of the most influential feature.

Table1. Variance Inflation Factor results.

Features names	***VIF***
Sequence of drop-casting (None/WS2/Perovskite)	3.278637
Drop casting(WS2/Perovskite)	1.643579
Perovskite(amount)	1.402285
$\mathbf{WS_2}$(amount)	3.677991

3. Results and Discussion

3.1. Prediction Model

Table 2 reports the evaluation results for each of the models. According to the evaluation results, XGBoost performed the best. Fig. 2 shows the actual values versus those predicted by the model in the whole data.

Table2. Performance of ML models for solar cell efficiency prediction.

Models	$\boldsymbol{R^2}$**(test/train)**	**RMSE(test/train)**
Random Forest	(0.87/0.9)	(0.07/0.04)
Gradient Boosting	(0.89/0.9)	(0.07/0.04)
XGBoost	(0.94/0.96)	(0.05/0.03)

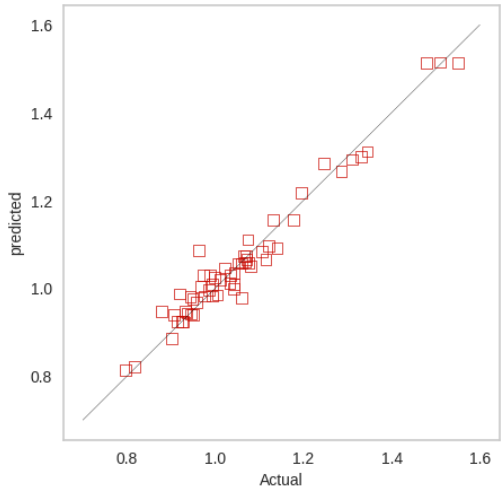


Fig 2. Actual values versus values predicted by the model.

This study aims to predict the solar cell's efficiency after the cell is coated with different concentrations of WS_2 and perovskite suspension to save time and cost. Therefore, to evaluate the performance of the trained model, 12 new data were used. Concentrations of 20 and 10 g/L perovskite with different numbers of drops were given to the model to predict the

relative efficiency of the cell. The table below reports the performance of the model on new data. The results indicate that the model is generalizable to new data.

Table3. Performance of the xgboost model for 12 new data.

Actual Value	Predicted Value	Material
1.076112896	1.068413	Perovskite(10 g/l)
1.075388480	0.980595	Perovskite(10 g/l)
1.034866436	0.946928	Perovskite(10 g/l)
0.983712584	0.971263	Perovskite(10 g/l)
0.964167685	0.988509	Perovskite(10 g/l)
0.991051390	0.992991	Perovskite(10 g/l)
0.949285623	1.068413	Perovskite(20 g/l)
0.952753803	0.980595	Perovskite(20 g/l)
0.959487465	0.946928	Perovskite(20 g/l)
0.958670306	0.971263	Perovskite(20 g/l)
0.938101288	0.988509	Perovskite(20 g/l)
0.945315659	0.992991	Perovskite(20 g/l)

3.2. Feature Importance Analysis

In the second step, only the XGBoost model was considered. The performance results of the model in training and testing are summarized in Table 4. The SHapley Additive exPlanation (SHAP) technique was used to investigate the contribution of each feature to the increase in solar cell efficiency.

Table4. Performance of ML models for solar cell efficiency prediction.

Models	R^2(test/train)	RMSE(test/train)
XGBoost	(0.79/0.8)	(0.093/0.063)

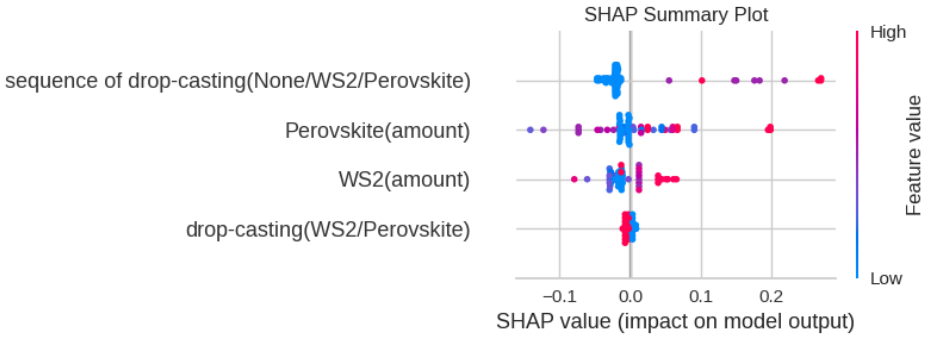


Fig 3. SHAP summary plot result for Xgboost model.

According to the SHAP summary plot in Figure 3, the presence of the second nanomaterial has a significant positive effect on the model output. Given that 1 and 2 represent perovskite and tungsten disulfide, respectively. Therefore, the red and purple dots in the SHAP summary plot represent tungsten disulfide and perovskite, respectively. Based on this, placing tungsten disulfide after perovskite on the cell surface has a greater positive effect on increasing cell efficiency than placing perovskite after tungsten disulfide.

4. Conclusion

In this work, we evaluated the ability of machine learning techniques to interpret the most influential features and predict the relative efficiency of a silicon solar cell after coating with certain concentrations of tungsten disulfide and perovskite. The XGBoost model performed well in predicting the relative efficiency of the cell. To evaluate the model's performance, 12 new data were given to the model. Comparing the actual values with the predicted values showed that the model can generalize to new data. In the second step, the most influential feature on the cell efficiency was investigated with SHAP. The greatest increase in efficiency occurs when WS_2 nanostructures are drop-cast after $CH_3NH_3PbBr_3$ perovskite nanostructures have been coated on the silicon solar cells. Overall, the findings of this study showed that the use of ML techniques can significantly help in optimizing experiments and saving time and cost, which facilitates the achievement of more efficient solar cells.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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