

## Highlights

### **Extracting the iron concentration in silicon solar cells using photovoltaic parameters and machine learning**

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- 80 ML models for iron quantification in silicon solar were tested
- XGB and DNN models outperform RF, GB, and SVR models
- MSE, MAPE, and R<sup>2</sup> reach up to 0.003, 3%, and 0.997 for synthetic data and 0.004, 9%, and 0.987 for experimental data

# Extracting the iron concentration in silicon solar cells using photovoltaic parameters and machine learning

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## ABSTRACT

Transitioning to renewable energy sources is paramount for humanity's sustainable development, and silicon solar cells are at the forefront of solar energy conversion. Iron in these structures is a primary one of the most detrimental metallic impurities. This study examines the impact of iron defect variability on silicon solar cell performance across various scenarios. We have simulated solar cells using SCAPS software across a range of temperatures (290 – 340) K, base thicknesses (180 – 380)  $\mu\text{m}$ , doping levels ( $10^{15}$  –  $10^{17}$ )  $\text{cm}^{-3}$ , with iron concentrations varying from  $10^{10}$  to  $10^{14}$   $\text{cm}^{-3}$  under AM1.5 and monochromatic (940 nm) illumination. Analyzed across all cases were the effects of iron-boron pair dissociation on short-circuit current, open-circuit voltage, fill factor, and efficiency. The experimental measurements validated the simulation results, demonstrating good agreement for all photovoltaic parameters. This study investigates the potential of using photovoltaic parameter changes induced by iron-related defect restructuring to estimate iron concentration. It is shown that changes in short-circuit current obtained under monochromatic illumination are the most reliable, while the fill factor is the least effective. The study examined the correlation between changes in photovoltaic parameters caused by pair dissociation while establishing the expedience of applying principal component analysis in impurity concentration evaluation with the help of multiple parameters.

## 1. Introduction

The urgent challenges of global warming and fossil fuel depletion have spurred the search for renewable energy sources, accelerating the rapid advancement of photovoltaic (PV) energy and the widespread deployment of solar panels [1, 2]. However, PV energy faces several significant challenges: the need to optimize solar cell manufacturing processes, improve the efficiency and stability of PV devices (either by discovering new materials or by enhancing existing structures), develop energy management systems designed to regulate the energy flow in real-time and establish methods for monitoring the condition of photoelectric converters, specifically through defect characterization. Simultaneously, the application of machine learning (ML) methods, which can identify patterns and correlations that are not readily apparent through traditional analysis [3], opens new avenues for addressing the issues above in photovoltaics. For instance, ML methods optimize individual production stages — such as crystal growth [4] and plasma-enhanced vapor deposition [5] — and streamline entire solar cell production lines, which may involve up to ten processing steps and forty-seven process parameter inputs [6]. Moreover, ML techniques enhance PV devices by identifying key photovoltaic materials, analyzing references to various structural configurations in the literature [7] or optimizing perovskite solar cells [8], designing renewable energy-based demand-side management systems [9], and extracting additional information from internal quantum efficiency measurements [10]. Numerous reviews provide further insights into ML applications in PV systems [11, 12, 13, 14, 15].

We will now explore the application of artificial intelligence in greater depth for defect analysis. Most relevant studies focus on image analysis of solar cells, including electroluminescence, photoluminescence, and infrared thermography [16, 17, 18, 19, 20, 21, 22, 23]. These methods facilitate detecting and classifying defects such as cracks, finger failures, hot spots, scratches, and horizontal dislocations and are predominantly implemented using convolutional neural networks. Another widely adopted approach involves applying ML models to current-voltage ( $I$ - $V$ ) curves, enabling the identification of permanent and temporal faults in PV arrays [24, 25, 26, 27]. A key advantage of this defect characterization method is its reliance on  $I$ - $V$  measurements, a standard procedure for PV device assessment. Additionally, ML techniques specifically designed for analyzing point defects warrant particular attention. For instance,

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researchers have developed methods for determining the electronic structure of intrinsic defects [28, 29], detecting radiation-induced defects via Raman spectroscopy [30, 31], and extracting recombination-active center parameters from temperature- and injection-dependent lifetime measurements [31, 32, 33]. Although such defects represent one of the main limitations of PV devices [34, 35], studies in this area remain scarce. Moreover, existing research primarily focuses on characterizing defects in PV materials rather than solar cells and relies on data obtained through specialized equipment.

This study proposes an ML-based approach to extract impurity concentrations from  $I-V$  curves. Specifically, we focus on quantifying iron in boron-doped crystalline silicon solar cells. This constraint is not overly restrictive, given that (i) Si-based solar cells dominate the current PV market [36, 37], with most being manufactured from boron-doped crystalline silicon (c-Si:B); and (ii) iron is one of the most prevalent, ubiquitous, and efficiency-limiting metallic impurities [38, 39]. It is well established that in *p*-type material, iron tends to bind with dopant atoms such as boron, forming iron–boron pairs under equilibrium conditions or existing as interstitial species only in the presence of sufficiently high free electron densities [40, 41]. The deliberate transition between these states can be readily induced through intense illumination, electron injection, or heating up to 200 °C and is commonly employed in various methods for assessing iron concentration [42, 43, 44, 45, 46, 47, 48, 49]. The approach proposed in this study leverages changes in photovoltaic parameters (PVPs) (short-circuit current, open-circuit voltage, efficiency, and fill factor) resulting from FeB dissociation as input features for ML algorithms. The specified PVPs can be easily extracted from  $I-V$  characteristics, making this method advantageous compared to existing approaches:

- (1) Unlike glow discharge mass spectrometry or secondary ion mass spectrometry [50], it is non-destructive;
- (2) It does not require specialized equipment or specially prepared samples, in contrast to Fourier-transform infrared spectroscopy, electron paramagnetic resonance, deep-level transient spectroscopy (DLTS), Laplace DLTS, carrier lifetime measurements, photoluminescence, or photoconductance [51, 52, 53, 43, 44, 47, 45];
- (3) It is relatively simple and fast compared to other methods that also rely on measuring PV parameters, such as the kinetics of short-circuit current [46] and open-circuit voltage [48], but require lengthy experimental procedures or multiple illumination levels.

In our previous work [54], we employed a deep learning approach to estimate iron concentration based on the ideality factor, which was also derived from  $I-V$  characteristics. However, the method proposed in this study imposes fewer constraints on the accuracy of  $I-V$  measurements across the entire voltage range and the model used to describe the  $I-V$  characteristics of actual structures. Thus, our approach allows for the simultaneous determination of iron impurity concentration along with key electrical parameters. These inline characterization techniques are crucial for ensuring efficient production lines and optimizing processes to produce reliable solar cells. Notably, luminescence imaging is increasingly used for solar cell characterization. However, ML methods have been proposed to extract  $I-V$  characteristic data from such images [55, 56]. Integrating these methods with our approach into a unified pipeline would enable the extraction of iron concentration data from luminescence measurements.

## 2. Methodology

The workflow of the ML pipeline for extracting iron contamination from IV data is shown in Fig. 1. A more detailed description follows.

### 2.1. Data Collection

Our research aimed to develop ML models for estimating iron concentration in silicon solar cells. Selecting relevant descriptors is a critical first step in building robust and effective predictive models. It is well established that the presence of iron induces the formation of recombination centers, which, in turn, affect the photoelectric conversion process and key PV parameters, including short-circuit current ( $I_{SC}$ ), open-circuit voltage ( $V_{OC}$ ), efficiency ( $\eta$ ), and fill factor ( $F!F$ ). Both theoretical and experimental studies [57, 39, 58] have demonstrated that the restructuring of iron-related defects (the dissociation of FeB pairs) leads to variations in PVPs that depend on iron concentration ( $N_{Fe}$ ). As a result, this investigation focused on using iron presence as a descriptor of the relative changes in PVPs caused by the  $Fe_iB_{Si} \rightleftharpoons Fe_i + B_{Si}$  reconstruction. Specifically, the relative changes in short-circuit current,  $\varepsilon I_{SC}$ , were calculated as

$$\varepsilon I_{SC} = \frac{I_{SC}^{FeB} - I_{SC}^Fe}{I_{SC}^{FeB}} \times 100\%, \quad (1)$$

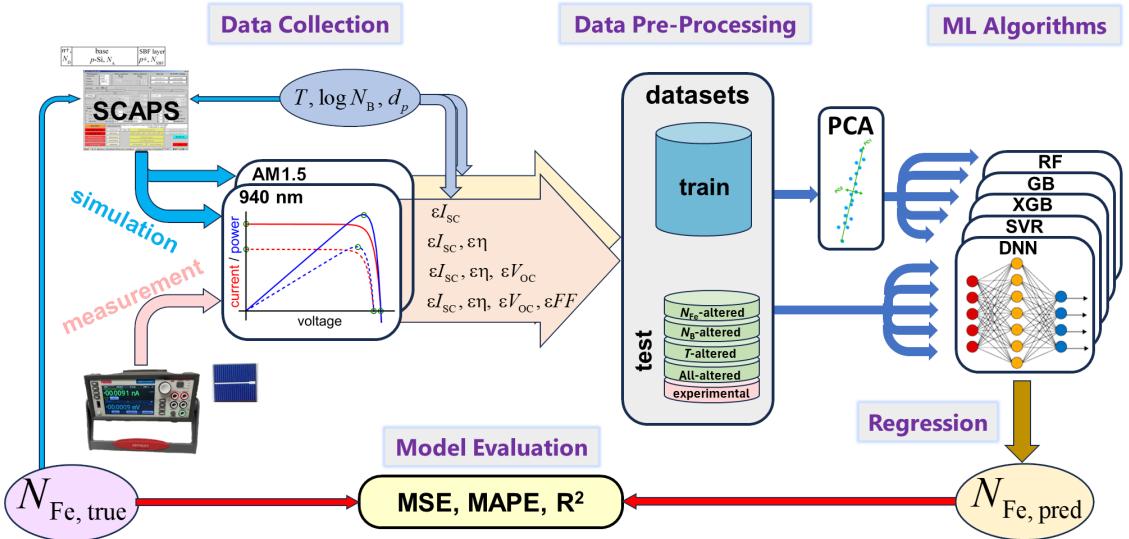


Figure 1: The workflow of the ML pipeline.

where  $I_{SC}^{FeB}$  and  $I_{SC}^{Fe}$  represent the short-circuit current values before and after pair dissociation, respectively. The relative changes in the other parameters ( $\varepsilon V_{OC}$ ,  $\varepsilon \eta$  and  $\varepsilon FF$ ) were determined similarly. Using relative rather than absolute changes helped, to some extent, isolate iron-related defect contributions from those of other recombination centers and mitigate potential fluctuations in external conditions, such as illumination intensity.

At the same time, changes in PVPs are shown [57, 58] to be influenced not only by iron concentration but also by specific characteristics of the solar cell structure, such as doping level and base thickness, as well as external factors, including temperature and illumination spectrum. Therefore, these effects must be considered when selecting an appropriate set of descriptors. In our study, we incorporated features such as boron concentration in the base ( $N_B$ ), base thickness ( $d_p$ ), and temperature ( $T$ ) and developed separate models for different illumination conditions.

For this research, datasets were obtained from both simulations and experiments. Specifically,  $I$ - $V$  curve simulations were performed for a silicon  $n^+$ - $p$ - $p^+$  structure using SCAPS 3.3.11. The SCAPS-1D software [59] is a widely used tool [60, 61, 62, 63, 64, 65] that enables modeling of barrier structure  $I$ - $V$  characteristics while accounting for defect states. PVPs were extracted from pairs of  $I$ - $V$  curves simulated for a solar cell with a known structure and a specified iron concentration under defined external conditions, both before and after FeB pair dissociation. This approach allowed us to determine the values of  $\varepsilon I_{SC}$ ,  $\varepsilon V_{OC}$ ,  $\varepsilon \eta$ , and  $\varepsilon FF$ . A detailed description of the modeling approach, including the used temperature dependencies of silicon and defect parameters, is provided elsewhere [66, 58].

To generate the training dataset, we performed simulations over a temperature range of (290 – 340) K for solar cells with a base thickness of (180 – 380)  $\mu\text{m}$ , a boron concentration of ( $10^{15}$  –  $10^{17}$ )  $\text{cm}^{-3}$ , and an iron concentration of ( $10^{10}$  –  $10^{14}$ )  $\text{cm}^{-3}$ . The simulations covered all parameter combinations within a four-dimensional grid, consisting of 11 values along the  $T$  axis, 5 along the  $d_p$  axis, 9 along the  $N_B$  axis, and 25 along the  $N_{Fe}$  axis. The values were evenly distributed within the specified ranges, with  $N_B$  and  $N_{Fe}$  spaced logarithmically. Each train dataset consisted of 12,375 samples obtained from simulations of 24,750  $I$ - $V$  characteristics.

We also generated four test datasets through simulation, each representing different scenarios that may arise in the practical application of ML models. In one test dataset, the iron concentration values used in the simulation were absent from the training set, while the other parameters ( $T$ ,  $d_p$ ,  $N_B$ ) matched the grid node values from the training simulations. This dataset was designated as “ $N_{Fe}$ -altered” and contained 1,034 samples. Similarly, we created the “ $N_B$ -altered” (1,100 samples) and “ $T$ -altered” (1,200 samples) test datasets using boron concentration and temperature values that were not present in the training dataset. In the “All-altered” dataset (1,190 samples), all four simulation parameters differed from those used in the training dataset.

The specified simulations for both the training and test datasets were performed under two lighting scenarios: AM1.5, which corresponds to standard characterization conditions for PV devices, and monochromatic light with a

wavelength of 940 nm and an intensity of  $5 \text{ W/m}^2$ , reflecting the remarkable sensitivity of PVPs to iron [58]. A total of 67,596  $I$ - $V$  curves were simulated.

For experimental validation of the proposed models, we used data obtained from measurements of real solar cells. We used a set of  $n^+$ - $p$ - $p^+$ -Si samples in the experiment. The structure was fabricated from a  $380 \mu\text{m}$  thick  $p$ -type boron-doped Czochralski silicon (100) wafer with a doping level of  $N_B = 1.36 \times 10^{15} \text{ cm}^{-3}$ . Iron concentration, determined using the methodology described in [67, 46], ranged from  $2 \times 10^{11}$  to  $4 \times 10^{13} \text{ cm}^{-3}$  across different samples. To create the experimental test dataset, we measured the  $I$ - $V$  characteristics under monochromatic illumination from a light-emitting diode (SN-HPIR940nm-1W) with a wavelength of 940 nm and an intensity of approximately  $5 \text{ W/m}^2$ , within a temperature range of (305 – 340) K. The decay of FeB pairs was induced using intensive halogen lamp illumination ( $7000 \text{ W/m}^2$ ). The number of samples in experimental dataset varied from 34 to 12, depending on the feature dimensionality.

## 2.2. Data Pre-Processing

Feature selection is a crucial pre-processing step in developing a forecasting model. Selecting the appropriate number of features requires balancing two competing factors. On one hand, fewer features simplify data collection and reduce computational costs. On the other hand, incorporating more features may enhance prediction accuracy by providing additional information. In this study, various feature combinations were explored. As shown in [58],  $\epsilon I_{SC}$  is a key metric for quantifying iron impurities due to its monotonic dependence on iron concentration and relatively large absolute values during the  $\text{Fe}_i\text{B}_{Si} \rightleftharpoons \text{Fe}_i + \text{B}_{Si}$  transformation. The following most suitable parameters for estimating  $N_{Fe}$  are  $\epsilon\eta$ ,  $\epsilon V_{OC}$ , and  $\epsilon FF$  [58].

Moreover,  $N_B$  (one of the selected descriptors) and  $N_{Fe}$  (target output) span several orders of magnitude. To achieve high prediction accuracy, we transformed the doping level and iron concentration into  $\log N_B$  and  $\log N_{Fe}$ . This approach is standard for quantities that vary over a wide range [68, 69].

Thus, we used the following sets to predict  $y = \log N_{Fe}$ :  $(T, d_p, N_B, \epsilon I_{SC})$ ;  $(T, d_p, N_B, \epsilon I_{SC}, \epsilon\eta)$ ;  $(T, d_p, N_B, \epsilon I_{SC}, \epsilon\eta, \epsilon V_{OC})$ ;  $(T, d_p, N_B, \epsilon I_{SC}, \epsilon\eta, \epsilon V_{OC}, \epsilon FF)$ . For simplicity, we will refer to the number of features as “dimension” from here on. That is, features with dimensions 4, 5, 6, and 7 were used in various models.

Data normalization transforms a dataset’s values to a standard scale, which can improve model accuracy. To standardize our features, we normalized them to have a mean of zero and a standard deviation of one.

Increasing the number of features does not always enhance informativeness if the descriptors are not independent. This study used the Pearson correlation coefficient to assess the relationships between input features. We found that changes in PV parameters are not entirely independent, particularly under monochromatic illumination (see Fig. S1 in the Supplementary Material). This is not surprising, since each of the PV parameters is linked to the diffusion and recombination of photo-induced charge carriers. Besides,  $\epsilon I_{SC}$ ,  $\epsilon V_{OC}$ ,  $\epsilon\eta$ , and  $\epsilon FF$  exhibit a strong correlation with boron concentration.  $N_B$  determines the position of the Fermi level, which, in turn, significantly influences the intensity of recombination processes within the Shockley–Read–Hall approximation. This provides the physical basis for the observed correlation.

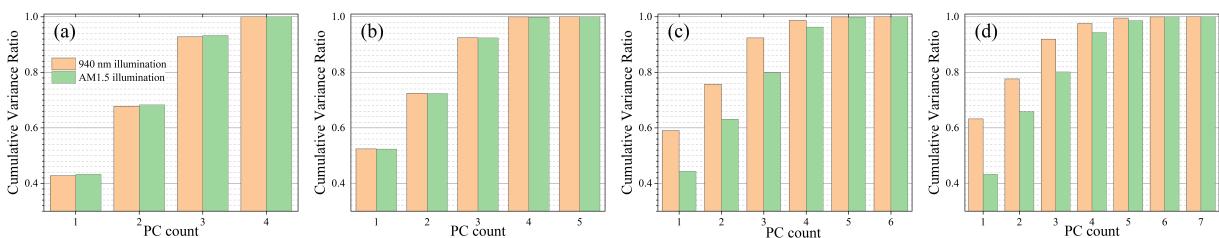
To ensure that ML algorithms are trained on independent input features while reducing data redundancy and memory usage, we applied Principal Component Analysis (PCA). PCA constructs new, uncorrelated features (principal components, PCs) and allows us to evaluate each PC’s contribution to the total variance. Fig.2 shows that increasing the feature dimension does not always enhance overall information variance. To assess the impact of redundant data, we trained ML models using features selected as follows: we computed PCs for the original dataset and then reduced the total dimension by discarding PCs whose contribution to the total variance was below 1.5%. The final dimensions of the different feature sets are provided in Table 1.

## 2.3. Machine Learning Algorithms

We used five ML algorithms to develop regression models for predicting iron concentration.

*Random Forest* (RF) improves predictive accuracy by training multiple decision trees on different subsets of the dataset. RF aggregates predictions from all trees using majority voting for classification or averaging for regression, reducing overfitting and increasing robustness to noise [70].

*Gradient Boosting* (GB) combines multiple weak learners, typically decision trees, to improve predictive performance. It sequentially adds predictors, with each new model correcting the errors of its predecessor, thereby enhancing overall accuracy. The final prediction is obtained by aggregating forecasts, usually through a weighted sum [71].



**Figure 2:** Cumulative explained variance versus number of PC components. Feature dimension: 4 (a), 5 (b), 6 (c), 7 (d).

**Table 1**

Feature dimension after PCA applying

Initial dimension	Final dimension	
	AM1.5 illumination	940 nm illumination
4	4	4
5	4	4
6	5	4
7	6	5

*eXtreme Gradient Boosting* (XGB) is an advanced ensemble method for gradient boosting machines [72]. Unlike standard GB, XGB utilizes the Newton–Raphson method with second-order derivatives of the loss function, improving accuracy, computational speed, and efficiency for large datasets.

*Support Vector Regression* (SVR) finds a hyperplane that maximizes the margin while minimizing errors within a specified tolerance. It maps input data into a high-dimensional feature space using kernel functions, effectively capturing nonlinear relationships [73].

*Deep Neural Network* (DNN) comprises multiple layers of interconnected neurons that process input data through successive nonlinear transformations [8].

It is worth noting that all the algorithms used have demonstrated effectiveness in previous defect studies [33, 32, 54, 14].

Considering different machine learning algorithms, data collected under various lighting conditions, features with varying dimensions, and the inclusion or exclusion of PCA, we evaluated 80 distinct models. From this point forward, the models will be referred to as

$$A_{\text{feat}}^{\text{illum}},$$

where “A” represents the ML algorithm used, and it can take one of the following values: (RF, GB, XGB, SVR, DNN); “illum” indicates the solar cell illumination type: illum ∈ (AM1.5, 940); “feat” represents the feature dimension and the application of PCA, where feat ∈ (4, 5, 6, 7, 4:PC, 5:PC, 6:PC, 7:PC).

The models are implemented using Python toolkits: Keras for DNN, Scikit-learn for RF, GB, and SVR, and XGBoost for XGB. Hyperparameter tuning is known [74] to be essential for optimizing model performance. We used the Optuna toolkit to optimize model parameters, employing the TPE sampler and Hyperband pruner for efficient hyperparameter selection. Tables S1–S5 (Supplementary Material) provide the tuned hyperparameters and their search ranges. It is worth noting that 5-fold cross-validation was employed during the model tuning process, with 20% of the train data used as the validation set to evaluate models trained on the remaining 80%. The chosen hyperparameter combinations are presented in Tables S6–S10.

## 2.4. Model evaluation

To build a regression model, it is crucial to evaluate its performance using various metrics. These metrics assess how well the model has learned and predicted outcomes. The evaluation metrics for iron quantification were the mean squared error (MSE), mean absolute percentage error (MAPE), and coefficient of determination ( $R^2$ ), as defined in

Eqs. (2)–(4).

$$\text{MSE} = \frac{1}{N} \sum_{i=1}^N (\hat{y}_i - y_i)^2, \quad (2)$$

where  $\hat{y}_i$  represents the predicted value for the  $i$ -th data point,  $y_i$  is the known value for the  $i$ -th data point, and  $N$  is the number of samples in the dataset. MSE is one of the most commonly used metrics for evaluating model accuracy. However, since the computation of  $\hat{y}_i$  involves the normalization and logarithm transformation of  $N_{\text{Fe}}$ , this metric does not fully reflect the accuracy of iron contamination estimation. Therefore, we used MAPE, which determines the mean relative error:

$$\text{MAPE} = \frac{1}{N} \sum_{i=1}^N \frac{|N_{\text{Fe,PRED},i} - N_{\text{Fe,TRUE},i}|}{N_{\text{Fe,TRUE},i}} \times 100\%, \quad (3)$$

where  $N_{\text{Fe,PRED},i}$  is the predicted value of iron concentration,  $N_{\text{Fe,TRUE},i}$  is the known value (used in simulation or obtained from experimental iron determination).

The  $R^2$  score is often interpreted as the percentage of explained variance and measures how well the predicted and true values align; a value of unity indicates a perfect prediction:

$$R^2 = 1 - \frac{\sum_{i=1}^N (N_{\text{Fe,TRUE},i} - N_{\text{Fe,PRED},i})^2}{\sum_{i=1}^N (N_{\text{Fe,TRUE},i} - \overline{N_{\text{Fe,TRUE}}})^2}, \quad (4)$$

where  $\overline{N_{\text{Fe,TRUE}}}$  is the mean of the true values.

In particular, Table S11 (Supplementary Materials) presents the performance metrics obtained using 5-fold cross-validation on the train dataset with the selected hyperparameter combinations.

The MSE and MAPE are highly sensitive to even a few low-accuracy predictions. To better assess the models and account for the impact of individual outliers, we also used the median absolute percentage error (MdAPE), which indicates the error value below which 50% of the predictions in the dataset fall. Furthermore, we evaluated the metric  $p$ , representing the percentage of samples (feature vectors) in a dataset with an absolute error below a specified threshold. Specifically, we computed the values of  $p_{01}$  and  $p_{10}$ , which represent the proportion of predictions in the dataset with an accuracy of 1% or better and 10% or better, respectively. The decrease in MdAPE and the increase in  $p_{01}$  and  $p_{10}$  indicate improved model performance due to a higher proportion of accurate predictions.

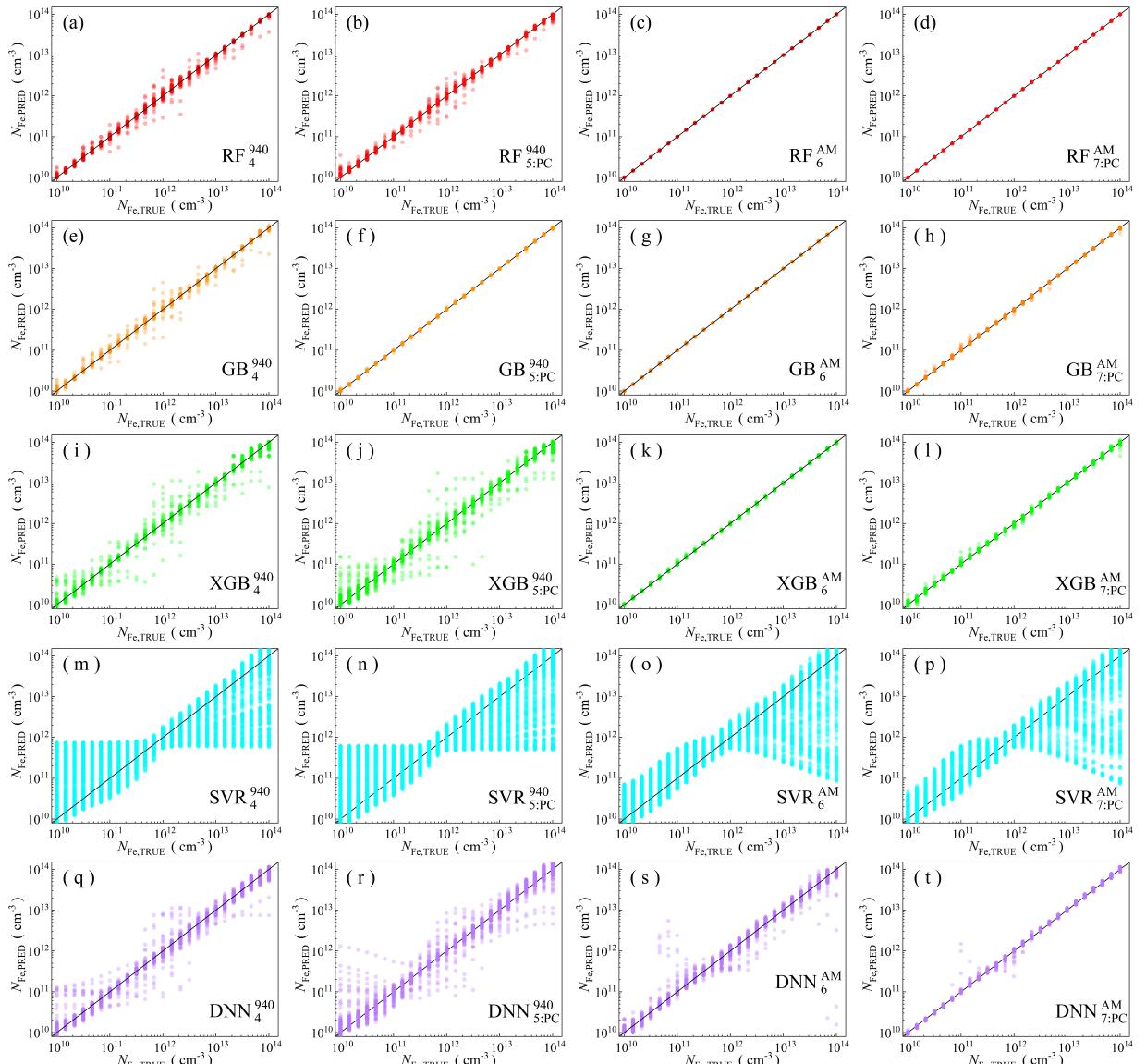
### 3. Results and Discussion

#### 3.1. Train dataset

Fig. 3 presents the models' prediction results on the training set. The Supplementary Materials (Figs.S4–S7) provide more detailed results, while Tables S12 and S13 list the performance metrics. The RF and GB models yield the most accurate predictions, whereas SVR performs the worst. Applying PCA generally reduces prediction accuracy on the training set.

As expected, increasing the number of descriptors enhances model performance (Fig. 4 and Fig.S7). The only exception occurs under AM1.5 illumination with PCA, where adding a fifth descriptor may degrade predictions rather than improve them. Overall, models trained on AM1.5 data exhibit significantly lower accuracy than those using monochromatic illumination, with errors approximately an order of magnitude higher. Notably, models with four descriptors (or five with PCA) under AM1.5 appear unpromising, even for RF and GB. Meanwhile, increasing the number of descriptors from six to seven offers little to no additional benefit in high-accuracy models such as RF, GB, XGB, and, to some extent, DNN.

Fig. 5 illustrates typical dependencies of the proportion of predictions with a given accuracy on  $T$ ,  $d_p$ ,  $N_B$ , and  $N_{\text{Fe}}$ , enabling an assessment of the models' predictive capabilities based on measurement conditions, solar cell structure, and iron concentration. The data indicate that the most challenging cases for prediction involve  $N_{\text{Fe}} < 10^{11} \text{ cm}^{-3}$  and



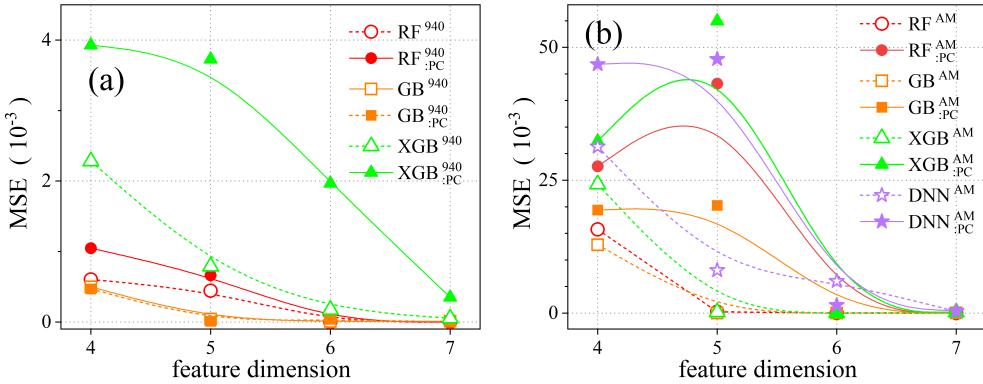
**Figure 3:** Scatter plots compare reference iron concentrations with ML-predicted values during the training phase. The ML algorithms include RF (a–d), GB (e–h), XGB (i–l), SVR (m–p), and DNN (q–t). The data come from simulation under monochromatic (a, b, e, f, i, j, m, n, q, r) and AM1.5 illumination (c, d, g, h, k, l, o, p, s, t). Panels b, d, f, h, j, l, n, p, r, and t include PCA. The input feature dimensions are 4 (a, e, i, m, q), 5 (b, f, j, n, r), 6 (c, g, k, o, s), and 7 (d, h, l, p, t). The black lines are the identified lines serving as the references.

solar cells with a base doping level around  $10^{16} \text{ cm}^{-3}$ . The last difficulty arises because, as shown by simulation [58], variations in PV parameters during FeB pair dissociation remain minimal. Meanwhile, measurement temperature and base thickness (when feature dimensionality exceeds 4) have virtually no impact on prediction accuracy.

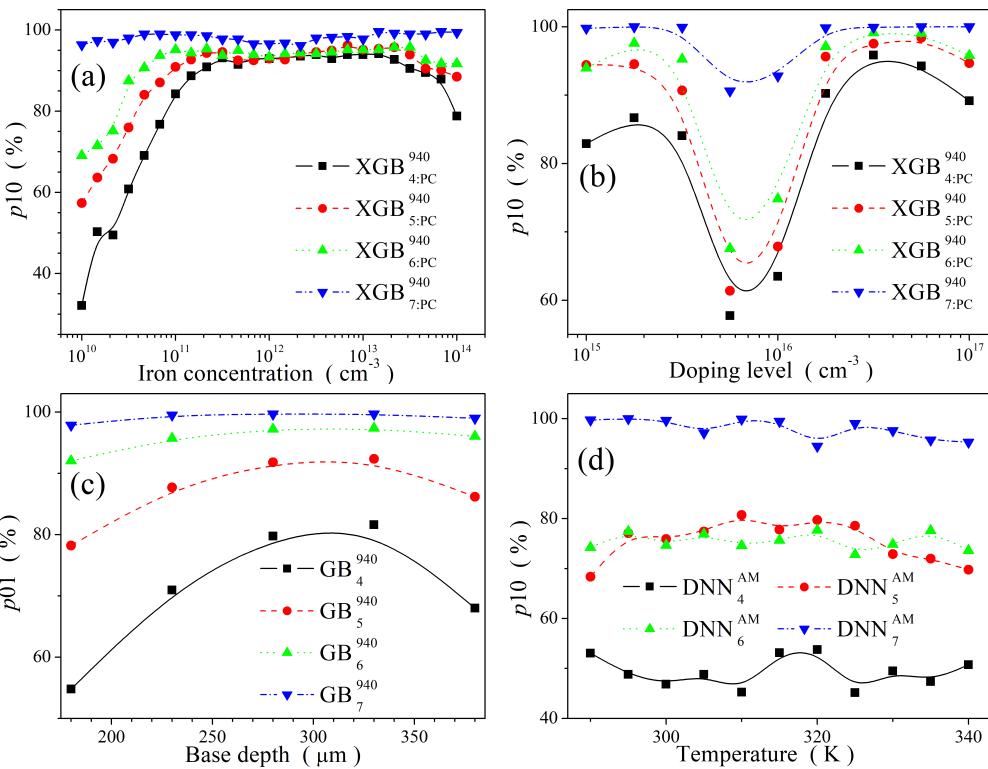
### 3.2. $N_{\text{Fe}}$ -altered test dataset

The  $N_{\text{Fe}}$ -altered test dataset simulates a practical scenario in which the goal is to predict iron concentration based on PVP variations measured under standardized conditions for predefined structures, using the same temperature and solar cell parameters as in model training.

Fig. 6 and Figs. S8–S11 present the prediction results, while Fig. 7 and Table 2 summarize the performance metrics. SVR consistently performs poorly, a trend observed across all test datasets. Since this pattern remains unchanged in

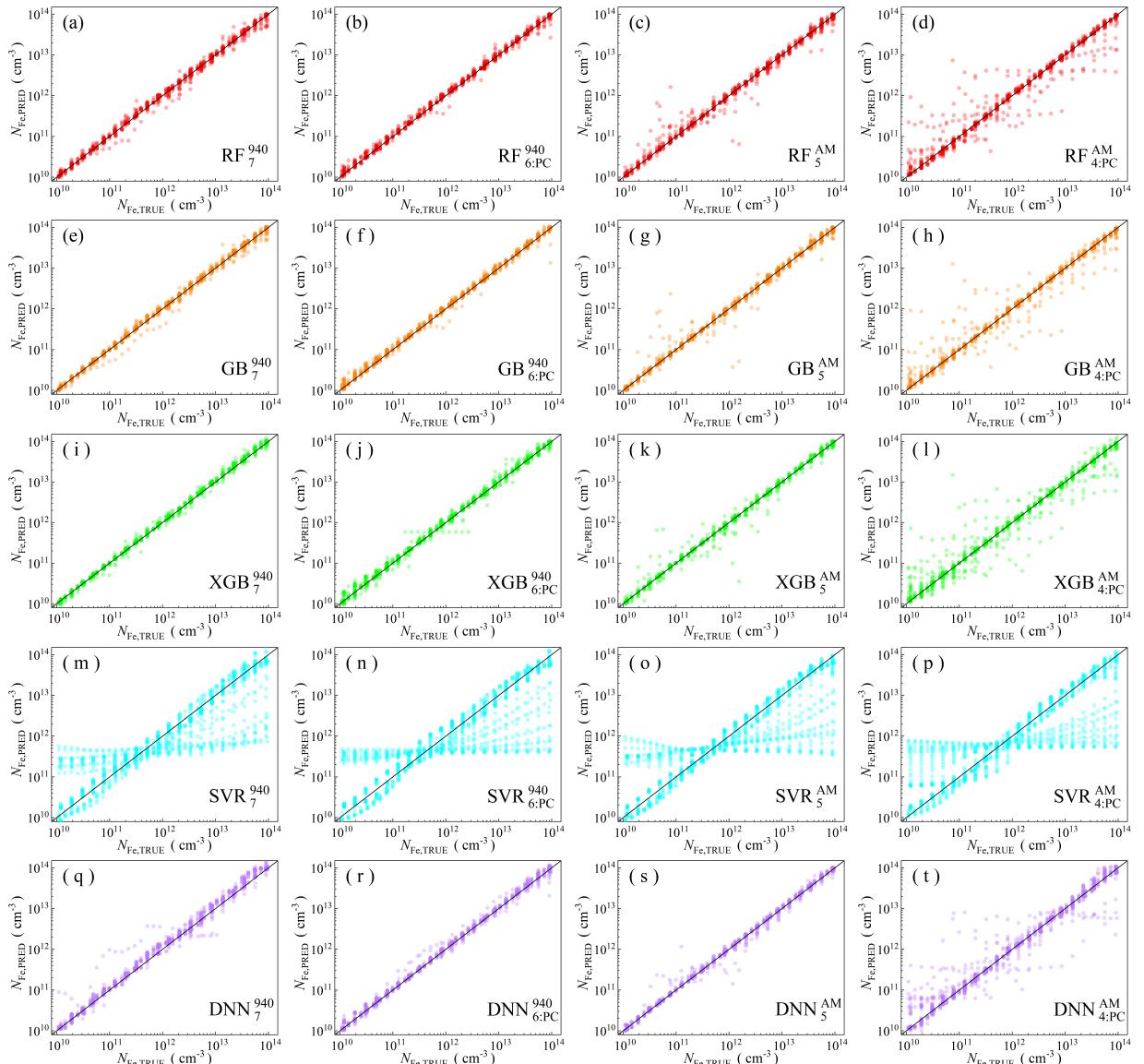


**Figure 4:** MSE dependence on input feature dimension for training data obtained under monochromatic (a) and AM1.5 illumination (b). ML algorithms: RF (circles), GB (rectangles), XGB (triangles), and DNN (stars). Closed markers indicate results with PCA, while open markers represent results without PCA.



**Figure 5:** Typical dependencies of the proportion of predictions with an accuracy of at least 10% (a, b, c) or 1% (d) on iron concentration, alloying level, substrate thickness, and temperature.

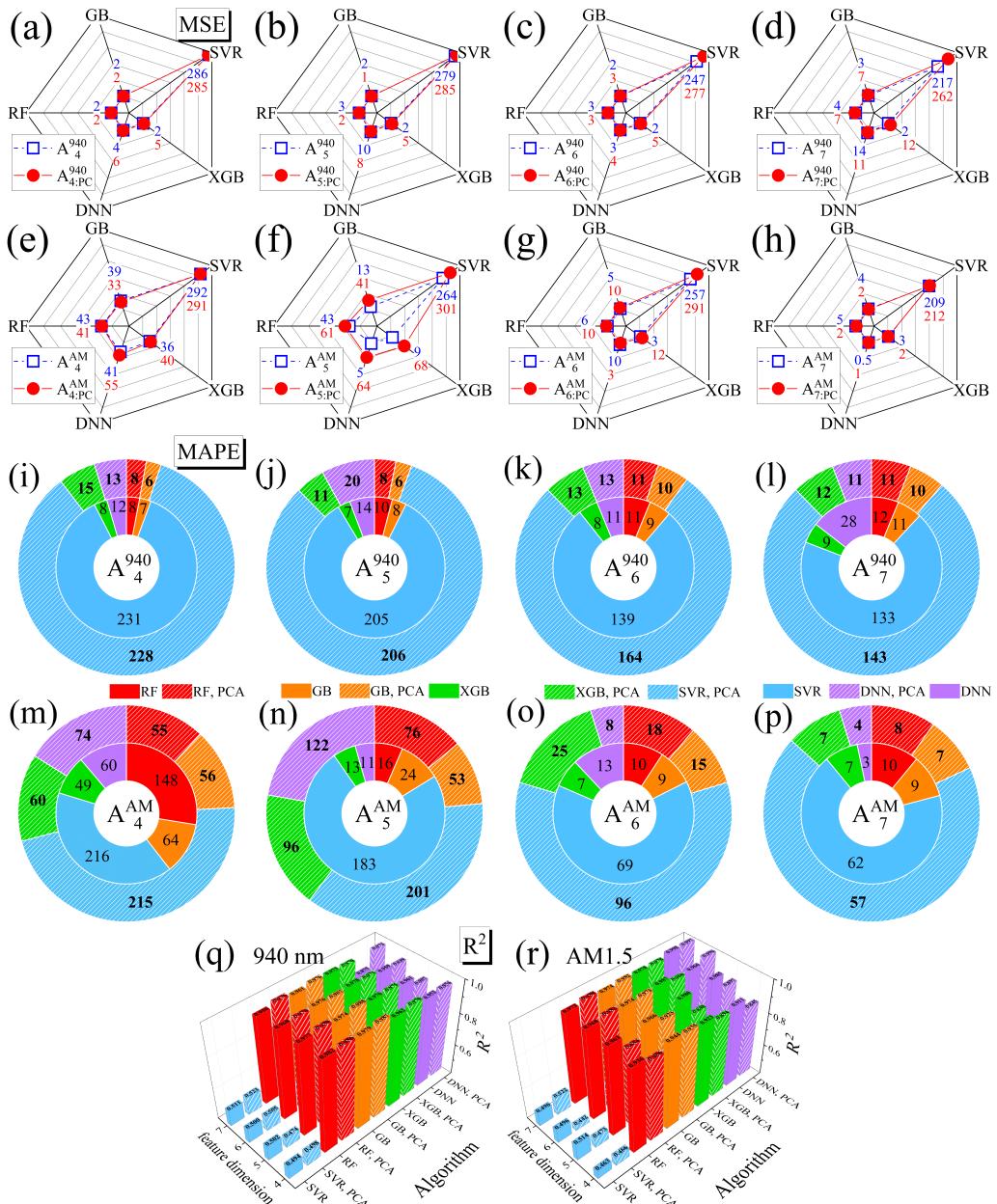
subsequent analyses, we do not discuss it further. For the remaining models, it is crucial to differentiate between results obtained under monochromatic and solar illumination. Under 940 nm illumination without PCA, nearly all algorithms achieve reasonably accurate predictions, with a MAPE of approximately 10DNN models yield slightly worse results, whereas XGB demonstrates marginally better performance. Interestingly, increasing feature dimensionality does not improve prediction accuracy but instead reduces it. Notably, incorporating the relative changes in the fill factor into the descriptor set significantly degrades DNN predictions. As shown in Table 2, RF, GB, and XGB, which are the most accurate models, exhibit a noticeable increase in MdAPE and a rise in p01 and p10 as the number of descriptors grows. These trends indicate that expanding feature dimensionality leads to a higher proportion of predictions with significant



**Figure 6:** Scatter plots compare reference iron concentrations with ML-predicted values during the  $N_{Fe}$ -altered test phase. The ML algorithms include RF (a-d), GB (e-h), XGB (i-l), SVR (m-p), and DNN (q-t). The data come from simulation under monochromatic (a, b, e, f, i, j, m, n, q, r) and AM1.5 illumination (c, d, g, h, k, l, o, p, s, t). Panels b, d, f, h, j, l, n, p, r, and t include PCA. The input feature dimensions are 7 (a, e, i, m, q), 6 (b, f, j, n, r), 5 (c, g, k, o, s), and 4 (d, h, l, p, t). The black lines are the identified lines serving as the references.

errors, as illustrated in Fig. 8,a for GB. Fig. 8,a and Table 2 also show that PCA-based model simplification increases the proportion of high-error predictions in XGB while reducing it in RF and GB. In summary,  $GB_{4:PC}^{940}$ ,  $GB_{5:PC}^{940}$ , and  $XGB_5^{940}$  yield the most precise results for this test dataset under monochromatic illumination, with the proportion of predictions achieving at least 10% accuracy reaching 80.3%, 82.4%, and 78.6%, respectively.

When estimating iron concentration based on PVP variations obtained under AM1.5 illumination, using only four descriptors does not yield sufficiently accurate predictions with any model. However, adding efficiency variations (increasing the feature dimension from 4 to 5) enables DNN and XGB to predict  $N_{Fe}$  with MAPE slightly above 10%, though the results remain inferior to those under monochromatic illumination. The use of PCA significantly worsens the results (see Fig. 7,f, Fig. 7,n, Table 2). A further increase in feature dimensionality improves prediction accuracy and



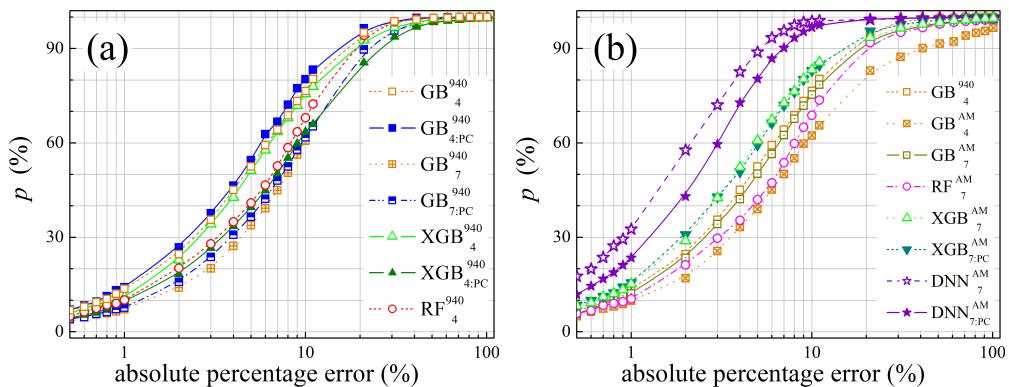
**Figure 7:** MSE (a–h), MAPE (i–p), and  $R^2$  (q, r) scores for various models, feature combinations, and illumination conditions on the  $N_{Fe}$ -altered test dataset. Illumination: 940 nm (a–d, i–l, q), AM1.5 (e–h, m–p, r). Feature dimensions: 4 (a, e, i, m), 5 (b, f, j, n), 6 (c, g, k, o), and 7 (d, h, l, p). Results with PCA are shown as circles (a–h) and shaded areas (i–r), while results without PCA are represented by squares (a–h) and filled regions (i–r). The numbers in panels (a–h) represent MSE values multiplied by 1000, while the numbers in panels (i–p) indicate MAPE values in percentage.

reduces the performance gap between models with and without PCA. The best results are observed when using seven descriptors. For RF and GB, applying PCA decreases both the mean errors (Fig. 7,p) and the proportion of predictions with large deviations from the true values (Table 2). For XGB and DNN — the most efficient models across the entire  $N_{Fe}$ -altered test dataset, including data under 940nm illumination — PCA provides no benefit (Fig. 7,p, Fig. 8,b). Notably, in these cases, the proportion of predictions with accuracy below 10% does not exceed 1.3%.

These results underscore the importance of selecting an optimal model and applying appropriate data preprocessing to achieve accurate iron concentration predictions in silicon solar cells.

**Table 2**Performance metrics of the ML models for  $N_{Fe}$ -altered dataset

Algorithm	Feature dimension	MdAPE (%)				p01 (%)				p10 (%)			
		940 nm		AM1.5		940 nm		AM1.5		940 nm		AM1.5	
		Init	PCA										
RF	4	6.47	6.38	8.29	8.00	10.1	9.48	7.54	8.12	68.0	70.2	57.0	57.9
	5	7.67	<b>6.00</b>	6.96	9.46	7.06	8.51	10.1	6.96	60.5	72.2	64.2	52.1
	6	8.01	7.34	5.46	5.66	6.58	7.74	11.0	10.9	59.5	60.4	72.4	72.9
	7	8.89	8.74	6.27	4.62	5.71	5.42	10.4	13.3	54.2	56.4	68.8	82.2
GB	4	4.63	4.35	6.95	6.27	<b>13.6</b>	<b>14.1</b>	9.87	9.38	76.5	80.3	62.4	67.2
	5	4.96	4.63	6.55	8.05	<b>13.6</b>	12.5	11.2	7.25	72.7	<b>82.4</b>	66.6	57.4
	6	6.78	6.73	5.31	4.41	8.03	9.09	11.9	15.4	65.5	64.0	74.4	79.1
	7	7.87	7.41	4.97	3.73	7.16	7.64	12.2	17.4	60.7	61.8	75.3	84.3
XGB	4	4.82	6.91	6.43	7.75	11.0	9.77	10.1	8.32	75.6	63.5	62.7	60.2
	5	<b>4.46</b>	6.20	4.26	9.04	11.7	10.2	13.8	6.58	<b>78.6</b>	68.6	74.7	52.3
	6	6.49	7.57	4.13	4.79	9.87	8.51	14.8	11.8	68.7	59.9	83.2	77.2
	7	6.16	7.96	3.71	3.94	8.80	7.54	15.2	15.6	66.0	60.9	83.3	83.0
SVR	4	31.1	26.7	41.2	40.5	1.45	1.35	1.06	0.77	14.9	18.2	11.4	11.8
	5	36.3	42.7	39.7	51.9	1.64	0.87	1.74	1.35	14.4	10.8	10.9	9.77
	6	37.0	44.8	37.3	44.2	1.16	0.48	1.64	0.77	13.4	8.99	14.4	10.1
	7	39.1	38.1	36.5	32.5	1.16	1.06	0.68	1.26	9.48	13.7	13.4	15.2
DNN	4	8.06	7.48	11.4	13.0	7.74	7.64	3.97	4.35	58.8	60.5	44.8	41.6
	5	7.42	9.02	5.97	6.84	6.48	6.67	10.1	6.77	66.0	54.7	72.3	61.4
	6	6.98	8.15	6.30	3.18	7.06	5.80	8.80	17.8	64.8	59.3	69.9	90.2
	7	17.3	6.93	<b>1.63</b>	<b>2.40</b>	4.06	8.90	<b>32.6</b>	<b>23.5</b>	33.1	64.7	<b>98.7</b>	<b>96.7</b>

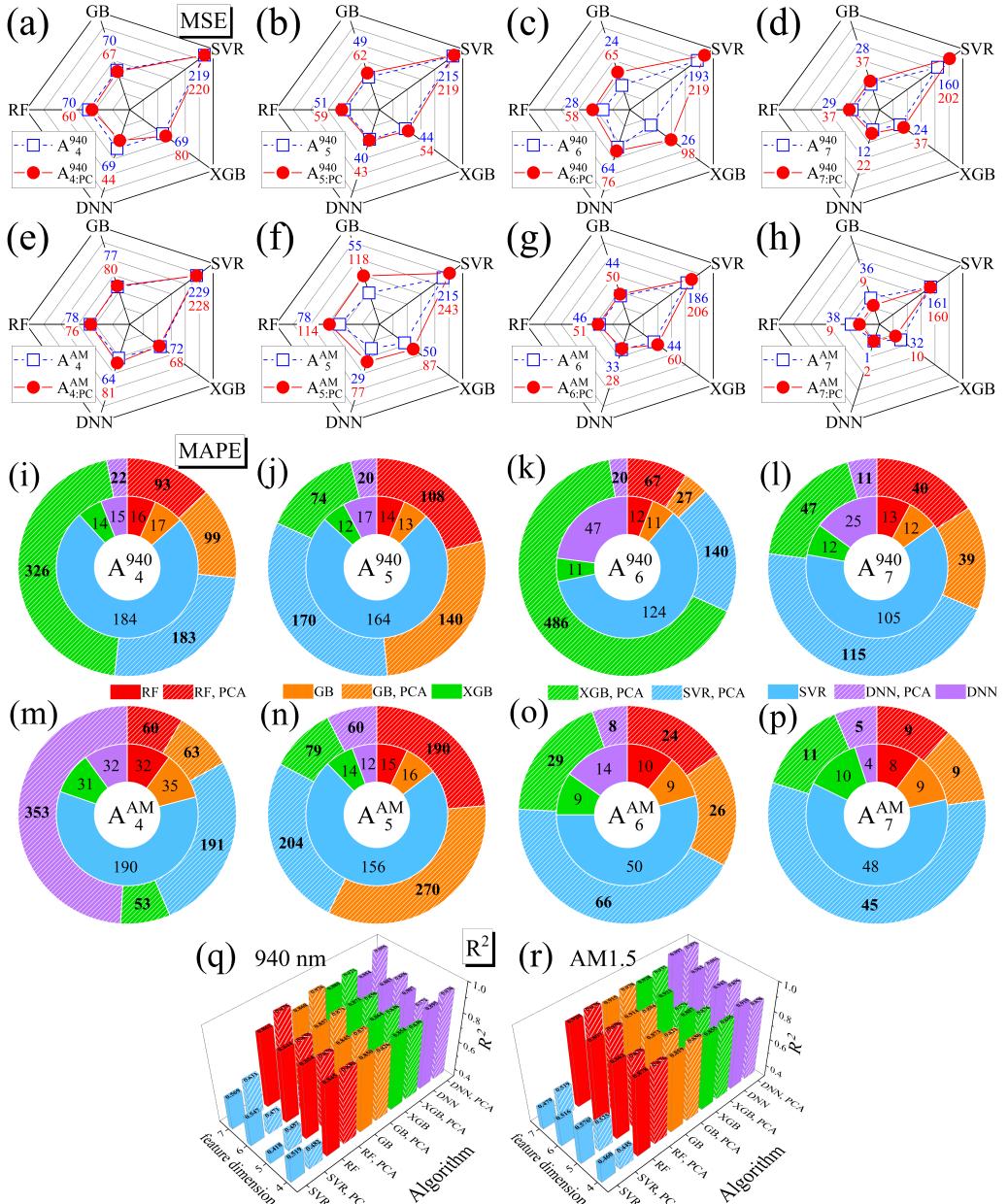
**Figure 8:** The proportion of samples in the  $N_{Fe}$ -altered dataset with an absolute error below a given threshold, plotted as a function of the threshold value.

### 3.3. $T$ -altered test dataset

The  $T$ -altered test dataset simulates a scenario in which impurity concentration estimates are based on measurements taken under conditions different from those used for model training. Additionally, this dataset includes temperature values (287 K, 341 K, and 342 K) that extend beyond the training range (290 – 340) K, enabling an assessment of the models' extrapolation capability.

Figs. S12–S15 present the prediction results, while Fig. 9 and Table 3 summarize the performance metrics. The data show that the average metrics for all models worsen slightly compared to the  $N_{Fe}$ -altered dataset (Fig. 7, Fig. 9). In most cases, PCA reduces model performance, except for AM1.5 at a feature dimensionality of 7. For the 940 nm case, using six descriptors proves more effective than using four, as observed in the previous test dataset.

A comparison of Table 2 and Table 3 reveals that, unlike the mean characteristics, MdAPE,  $p01$ , and  $p10$  are often better than those in the  $N_{Fe}$ -altered dataset. For example, for  $XGB_6^{940}$ , MdAPE and  $p01$  reach 2.47% and 33.6%,



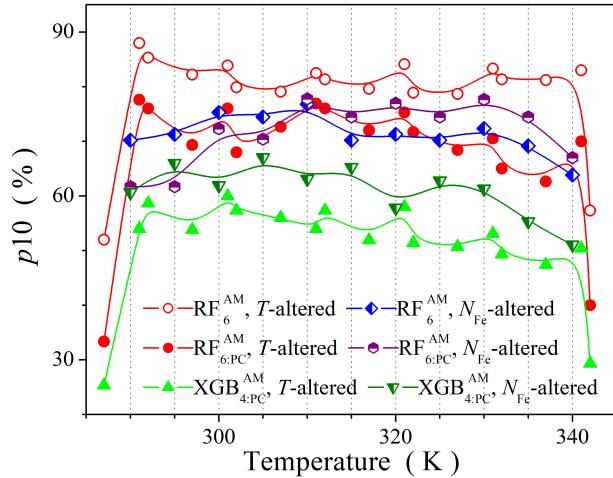
**Figure 9:** MSE (a–h), MAPE (i–p), and  $R^2$  (q, r) scores for various models, feature combinations, and illumination conditions on the  $T$ -altered test dataset. Illumination: 940 nm (a–d, i–l, q), AM1.5 (e–h, m–p, r). Feature dimensions: 4 (a, e, i, m), 5 (b, f, j, n), 6 (c, g, k, o), and 7 (d, h, l, p). Results with PCA are shown as circles (a–h) and shaded areas (i–r), while results without PCA are represented by squares (a–h) and filled regions (i–r). The numbers in panels (a–h) represent MSE values multiplied by 1000, while the numbers in panels (i–p) indicate MAPE values in percentage.

whereas in the previous case, the best values were 4.46% and 13.6%. These differences in the behavior of MSE, MAPE, and  $R^2$ , compared to other performance metrics, suggest a higher proportion of accurate predictions while increasing error values in less successful forecasts. In other words, prediction disparity increases — the rich get richer, and the poor get poorer.

Fig. 10 illustrates the dependence of the proportion of predictions with an error below 10% on temperature for the two training datasets. Within the (290–340) K range, where the networks were trained, both datasets exhibit similar  $p_{10}$  values and overall trends, despite the temperature values in the  $T$ -altered test dataset differing from those used during

**Table 3**Performance metrics of the ML models for  $T$ -altered dataset

Algorithm	Feature dimension	MdAPE (%)				p01 (%)				p10 (%)			
		940 nm		AM1.5		940 nm		AM1.5		940 nm		AM1.5	
		Init	PCA										
RF	4	6.50	13.1	<b>1.88</b>	11.6	18.2	8.92	<b>28.1</b>	11.8	60.4	40.8	<b>95.6</b>	45.2
	5	5.59	13.2	9.58	5.90	22.4	6.75	12.1	16.6	62.9	40.7	51.3	62.7
	6	4.61	13.3	14.2	2.13	20.8	8.58	9.50	35.3	68.8	43.5	42.1	77.3
	7	5.07	9.82	5.05	<b>1.94</b>	21.5	12	17.7	38.7	67.4	50.4	68.3	79.8
GB	4	5.29	12.5	3.47	10.1	20.7	6.67	21.5	5.08	62.0	42.9	80.6	49.8
	5	4.91	12.6	9.34	4.89	19.1	7.00	6.58	22.5	66.2	44.7	51.8	65.0
	6	3.41	9.12	12.8	1.81	22.3	11.2	4.67	<b>40.9</b>	73.1	52.4	43.2	78.3
	7	5.03	9.72	5.14	2.44	15.6	10.2	13.9	31.3	68.3	51.0	70.7	79.3
XGB	4	5.03	10.9	3.40	8.72	22.8	8.92	20.8	8.42	64.6	46.9	80.8	53.8
	5	3.64	9.01	9.88	5.14	28.4	8.75	7.00	23.7	67.3	53.0	50.3	66.3
	6	<b>2.47</b>	10.4	10.5	2.08	<b>33.6</b>	6.75	6.58	34.4	<b>73.7</b>	49.2	48.6	78.0
	7	9.93	<b>5.37</b>	5.78	3.38	9.92	<b>14.9</b>	12.3	19.3	50.3	<b>67.9</b>	69.2	78.3
SVR	4	30.9	27.8	5.11	36.4	1.50	1.58	13.6	0.67	15.3	18.3	72.9	12.8
	5	33.7	38.0	35.7	37.5	1.75	1.00	1.17	0.92	15.3	12.9	13.5	12.8
	6	38.3	40.9	47.6	37.1	1.50	1.50	0.67	1.25	14.3	15.0	9.83	12.8
	7	18.6	6.85	46.2	36.3	3.83	7.50	0.75	1.83	29.8	66.3	9.58	15.4
DNN	4	6.92	7.54	10.5	14.2	7.83	8.33	4.58	4.67	65.3	59.0	47.3	37.2
	5	6.53	8.90	5.46	7.44	9.17	5.50	10.9	7.42	68.8	53.8	71.6	58.4
	6	7.09	7.18	4.92	2.99	7.50	9.25	10.7	18.3	66.8	61.1	79.2	90.9
	7	39.3	35.9	32.2	2.53	1.25	1.50	1.00	23.2	10.7	13.3	14.7	<b>92.5</b>

**Figure 10:** Typical dependencies of the fraction of predictions with an accuracy within 10% as a function of temperature for the  $T$ -altered and  $N_{Fe}$ -altered datasets.

training. Specifically,  $p10$  remains nearly independent of temperature, consistent with the trend observed in Fig. 5d. However, a slight deviation of just a few kelvins from the training range significantly reduces prediction accuracy. This behavior highlights the models' limited extrapolation capability compared to their interpolation performance. The degradation of the average metrics (MSE, MAPE,  $R^2$ ) primarily results from lower prediction accuracy at temperatures beyond the training range.

### 3.4. $N_B$ -altered and All-altered test datasets

### 3.5. Experimental validation

## 4. Conclusion

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## Supplementary data

Supplementary data to this article can be found online at <http://surl.li/qneich>

## Data availability

Data will be made available on request.

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