# Machine Learning-Based Characterization of Recombination Active Defects in Photovoltaic Cells

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The application of artificial intelligence, particularly machine learning (ML), in renewable energy research is gaining traction [1]. Recent studies increasingly employ photoluminescence spectroscopy and ML to investigate defect recombination in solar cells (SC). However, the majority of these studies are not specifically related to point defects. Our study aims to develop a cost-effective ML-based approach for characterizing point defect in silicon SC using I-V measurements.

To showcase our methodology, we focused on assessing the concentration of iron-related defects (Fei and FeiBs). Using SCAPS-1D software, we modeled SC characteristics under standard AM1.5 and monochromatic (940 nm) illuminations. The modeled I-V curves provided insight into iron impurity states, allowing us to derive relative changes in short-circuit current (εIsc), open-circuit voltage (εVoc), efficiency (εη), and fill factor (εFF) post FeiBs pairs decay. ML methods, including deep neural networks (DNN), random forest (RF), and gradient boosting (GB), were employed to estimate iron concentration. Prediction accuracy was compared across different lighting conditions and descriptor numbers, encompassing base depth, doping level, temperature, εIsc, εη, εVoc, and εFF. Results are presented in Table 1.

*Table 1. Accuracy of iron concentration prediction for test dataset*

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Algorithm | Number of descriptors | MSE (10-3) | | MRE (%) | | R2 | |
| illumination | | | | | |
| AM 1.5 | 940 nm | AM 1.5 | 940 nm | AM 1.5 | 940 nm |
| DNN | 4 | 49 | 10 | 115 | 14 | 0.924 | 0.972 |
| 5 | 5 | 4 | 13 | 8 | 0.991 | 0.981 |
| 6 | 2 | 3 | 8 | 9 | 0.993 | 0.899 |
| 7 | 0.6 | 2 | 3 | 9 | 0.998 | 0.977 |
| RF | 4 | 41 | 2 | 83 | 8 | 0.939 | 0.982 |
| 5 | 10 | 3 | 16 | 10 | 0.963 | 0.977 |
| 6 | 5 | 3 | 10 | 11 | 0.971 | 0.968 |
| 7 | 5 | 4 | 10 | 12 | 0.975 | 0.956 |
| GB | 4 | 41 | 2 | 66 | 7 | 0.949 | 0.978 |
| 5 | 12 | 2 | 18 | 8 | 0.966 | 0.969 |
| 6 | 5 | 2 | 9 | 9 | 0.970 | 0.973 |
| 7 | 4 | 3 | 9 | 11 | 0.981 | 0.959 |

1. Dwivedi P., Weber J. W., Lee Chin R., Trupke T., Hameiri Z. Deep learning method for enhancing luminescence image resolution. *Solar Energy Materials and Solar Cells*. 2023. V.257, P. 112357.