

## Highlights

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

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- The iron defect transformation effect on Si solar cells' performance was studied using SCAPS simulation
- Short-circuit current changes are most suitable for estimating iron impurity concentration.
- Open-circuit voltage changes are a non-monotonic function of iron concentration at low doping levels.
- Monochromatic illumination is more effective than AM1.5 for accurate iron concentration estimation.

# 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.

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## 1. Introduction

[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44? ]

## 2. Research Methodology

### 2.1. Simulation Details

## 3. Results and Discussion

## 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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