Dear Editor and Reviewers,

We sincerely thank you for taking the time to review our manuscript "Iron's impact on silicon solar cell execution: comprehensive modeling across diverse scenarios" (Ms. Ref. No.: MSB-S-24-02710). Your insightful comments and constructive suggestions have greatly helped us improve the quality of our work. We particularly appreciate your careful reading and thoughtful feedback, which have led to significant improvements in both the technical content and presentation clarity of our manuscript. We have carefully addressed all the comments and made corresponding revisions to the manuscript. Below we provide our detailed point-by-point responses to each comment. We hope the revised manuscript better meets your expectations and standards for publication in Materials Science and Engineering: B.

## Response to Reviewer #1

**Comment 1.** *The author must explain the specific mechanisms you propose for the interaction between iron-related defects and other impurities in silicon solar cells? How might these interactions complicate the interpretation of photovoltaic performance metrics?*

**Reply:**

In general, interstitial iron is already mobile at room temperature and can interact with various impurities. Over 30 iron-related complexes have been identified in silicon, and nearly 25 energy levels associated with iron-related defects have been reported in the silicon bandgap across different studies [1, 2, 3]. For example, iron forms complexes with carbon, oxygen, hydrogen, sulfur, and other metal impurities, as well as with native defects in silicon. However, in terms of their impact on photovoltaic performance, two primary factors must be considered. First, the concentration of the relevant defects is crucial. It is widely recognized that in $p$–type silicon under equilibrium conditions, most iron impurity atoms pair with acceptors (e.g., boron in Si:B) [4, 1]. The concentration of other complexes is significantly lower, and detailed investigation of these complexes requires specialized sample preparation, such as additional doping with other expected complex components or irradiation to increase the concentration of native defects [5]. Further supporting this, several methods used to evaluate the total iron concentration in $p$–Si rely on breaking the FeB pair [6, 7, 8]. Second, the recombination activity of these centers must be considered, as it depends on the defect energy level relative to the Fermi level and the charge carrier capture cross-section. Interstitial iron and FeB pairs are among the most detrimental recombination-active impurities in $p$–Si [1, 9] in contrast to other iron-related defects. Notably, iron gettering by oxygen precipitates or structural defects increases carrier lifetime [10, 11]. In $n$–Si, $Fe_i$ is not a recombination-active impurity due to the filling of its energy level. Reducing the impact of iron through gettering during phosphorus diffusion [10, 11, 12] or the formation of a passivating layer [13] is well-established and used in the solar cell industry.

Thus, our assumption that the primary influence of iron impurities in the $p$–regions of a solar cell on photoelectric parameters is due to $Fe_iB_{Si}$ pairs and $Fe_i$ is fully justified. Furthermore, we emphasize that this paper focuses on the relative changes in parameters during $Fe_iB_{Si} \rightleftarrows Fe_i + B_{Si}$ transformation, which enables the isolation of these specific defects' contributions.

This answer is incorporated in the revised text on page 5, two last paragraph in Section 2.1. Simulation Details.

**Comment 2.** *The author should give the transient nature of defect dynamics, how do you assess the long-term stability of silicon solar cells in the presence of iron contamination? What experimental approaches would you recommend to study the aging effects of these defects over time?*

**Reply:**

Interstitial iron atoms exhibit high mobility in silicon [1]. For example, the characteristic time required for FeB pair formation, which depends on the diffusion coefficient of $Fe_i$, is given by the following expression [14, 15, 16]:

$$\tau = 5.7 \times 10^5 \, \frac{s}{K \, cm^3} \times \frac{T}{N_B} \exp\left(\frac{0.65}{kT}\right).$$

$$(1)$$

where $N_B$ is the doping level.

That is, at room temperature, the formation of an equilibrium concentration of FeB pairs is completed within 24 hours, while at $T = 340$ K, the $\tau$ is approximately 10 minutes. Therefore, iron contamination is not a determining factor in the long–term stability of silicon solar cells, unlike sodium atoms, which are considered one of the primary contributors to potential-induced degradation [17].

The information on the characteristic time of FeB pair formation has been added to the revised manuscript (page 5, last paragraph in Section 2.2.).

> The measurements were carried over the temperature range of 300-340 K. The sample temperature was driven by a thermoelectric cooler controlled by an STS-21 sensor and maintained constant by a PID algorithm embedded in the software that serves the experimental setup. Notably, the characteristic time for FeB pair recovery after the cessation of illumination is approximately 13,000 seconds at 300 K and only 600 seconds at 340 K [14, 15]. These limitations affect the measurement duration at high temperatures, and the experiments accounted for them.

**Comment 3.** *An Author should provide a theoretical framework for understanding how the temperature range you studied (290 K to 340 K) influences the activation energy of iron-related defects? How might this affect the performance of solar cells in varying environmental conditions?*

**Reply:**

Initially, we note that the selected temperature range reflects the realistic operating conditions of most silicon solar cells. In our calculations, we accounted for the temperature dependencies of both silicon properties — including bandgap, the effective density of states; effective masses, thermal velocities and mobilities of charge carriers; Auger and band-to-band recombination coefficients, and light absorption values — and defect parameters, such as energy level positions within the bandgap and electron and hole capture cross-sections. Additionally, we considered the temperature dependence of the equilibrium concentration ratio of $Fe_i$ and FeB. Specifically, the primary effect of increasing temperature on iron-related defects is the rise in the relative equilibrium concentration of interstitial iron atoms and the change in the charge carrier capture cross-section of each defect.

Accounting for all the above factors in the modeling process suggests that the results presented in this work accurately reflect the impact of both defects and defect parameter variation on solar cell performance under varying environmental conditions, including temperature, illumination type, and intensity.

Details on how temperature dependencies were accounted for in the simulation can be found on page 3, last two paragraphs

> As can be seen from Table 1, calculations spanned a broad range of temperatures and base doping levels. Therefore, to improve the accuracy of the calculations when inputting the initial parameters into SCAPS, temperature and concentration (where applicable) dependencies of the following silicon parameters were taken into account:
> - bandgap according to Passler [18];
> - doping induced bandgap narrowing according to Yan & Cuevas [19];
> - effective density of states at conduction and valence band and intrinsic carrier concentration according to Couderc et al. [20];
> - thermal carrier velocities according to Green [21];
> - free carrier effective masses according to O'Mara et al. [22];
> - carrier mobilities according to Klaassen's theory [23];
>
> The values of surface recombination coefficients were considered equal to the thermal velocities of carriers [24]. The calculations addressed recombination processes within the structural volume, incorporating both intrinsic recombination and Shockley-Read-Hall (SRH) recombination at iron-related defects. In the first case, processes of band-to-band radiation recombination were considered (where the calculation of the corresponding coefficient included the fraction of radiatively emitted photons reabsorbed via band-to-band processes according to Niewelt et al.[25]) and Auger recombination (where the coefficients considered the effect of Coulomb enhancement [26] and temperature dependence [27]).

and page 4, 3rd and 4th paragraph from the top

Case 2. Iron atoms predominantly form pairs with acceptors, $\left[\text{Fe}_i\text{B}_s\right] \gg \left[\text{Fe}_i\right]$, but the exact concentration ratio depends on the position of the Fermi level and temperature [28, 29] and varies from point to point within the solar cell. Further details about calculation of the concentration profiles of $\text{Fe}_i\text{B}_s$ and $\text{Fe}_i$ are provided in [30, 31]. This case corresponds to prolonged storage of the structure in darkness or under conditions of low-intensity ($< 0.01$ J cm$^{-2}$ [32]) illumination.

During the calculations, it was assumed that $\text{Fe}_i$ forms a single donor level, while the $\text{Fe}_i\text{B}_s$ pair has a trigonal configuration and acts as an amphoteric defect. We obtained defect parameters, including energy level positions within the bandgap, electron and hole capture cross-sections, and their temperature dependencies, based on data from relevant studies [33, 1, 34].

**Comment 4.** *An Author mentioned the application of principal component analysis in evaluating impurity levels. Could you elaborate on how this technique was implemented in your study and its effectiveness in distinguishing between different types of impurities?*

**Reply:**

One of the objectives of this study was to evaluate the feasibility of using variations in short-circuit current, open-circuit voltage, solar cell efficiency, or fill factor, which results from the decay of iron-containing pairs, to estimate the concentration of iron impurities. Our simulations revealed that the relative changes in these parameters depend not only on the iron concentration but also on temperature and other solar cell characteristics, such as doping level and base thickness. In other words, when determining the magnitude of $N_{\text{Fe}}$ based on changes in short-circuit current, a set of parameters (descriptors) must be used: $(T, d_p, N_{\text{B}}, \varepsilon I_{\text{SC}})$. Evidently, incorporating additional information, such as changes in efficiency ($\varepsilon\eta$), along with an expanded set of descriptors $(T, d_p, N_{\text{B}}, \varepsilon I_{\text{SC}}, \varepsilon\eta)$, increases the complexity of calculations due to the growing number of input parameters. However, this should enhance the accuracy of $N_{\text{Fe}}$ predictions. Meanwhile, variations in short-circuit current and efficiency are not entirely independent, as both essentially characterize the same physical process — the diffusion of photo-induced carriers. Confirmation of this has resulted from analyzing the correlations between parameters — see Fig. 12 in the manuscript. Thus, the set $(T, d_p, N_{\text{B}}, \varepsilon I_{\text{SC}}, \varepsilon\eta)$ contains useful and redundant information compared to $(T, d_p, N_{\text{B}}, \varepsilon I_{\text{SC}})$. To assess the degree of redundancy in different descriptor sets, we employed principal component analysis (PCA), which constructs a new dataset of uncorrelated principal components (PCs). PCA also enables the evaluation of each PC's contribution to the total variance of the information. Our analysis showed that, for example, when estimating $N_{\text{Fe}}$ using a set of seven descriptors $(T, d_p, N_{\text{B}}, \varepsilon I_{\text{SC}}, \varepsilon\eta, \varepsilon V_{\text{OC}}, \varepsilon FF)$ obtained under 940 nm illumination, five PCs account for more than 99.5% of the variance in the input data. Therefore, applying PCA to transform the seven input variables and using only five is fully justified, as it significantly simplifies calculations with minimal impact on estimation accuracy.

In the manuscript, PCA was not used to evaluate impurity levels. The conclusions and abstract only mentioned its potential usefulness in estimating the concentration of iron impurities based on variations in several photovoltaic parameters. We apologize for any possible ambiguities in the wording. In the revised manuscript, we have aimed for the most precise formulations. Finally, we would like to thank the Reviewer for an idea about PCA use to distinguish the contributions of different defects in future research.

The corrections were made in the manuscript on page 15, 1st paragraph in Section 3.5.

The previous subsections demonstrated that by using the relative changes in photovoltaic energy conversion parameters following the dissociation of FeB pairs (e.g., changes in short-circuit current), along with considering solar cell parameters (such as base depth and doping level) and measurement conditions (such as temperature and illumination type), it is possible to predict iron concentration. One approach to evaluating the value of $N_{\text{Fe}}$ is to apply a machine learning algorithm (random forest, gradient booster, or artificial neural network etc.). If we assume that the training process is conducted separately for each illumination variant and want to determine the magnitude of $N_{\text{Fe}}$ based on changes in short-circuit current, the input set of descriptors could be $(T, d_p, N_{\text{B}}, \varepsilon I_{\text{SC}})$. Evidently, incorporating additional information, such as changes in efficiency ($\varepsilon\eta$), along with an expanded set of descriptors $(T, d_p, N_{\text{B}}, \varepsilon I_{\text{SC}}, \varepsilon\eta)$, increases the complexity of calculations due to the growing number of input parameters. However, this should enhance the accuracy of $N_{\text{Fe}}$ predictions. At the same time, when comparing Fig. 3 and Fig. 10, it is clear that $\varepsilon I_{\text{SC}}$ and $\varepsilon\eta$ are not entirely independent. This outcome is understandable

from a physical standpoint as short-circuit current and efficiency characterize the same physical process — the diffusion of photo-induced carriers. Thus, the set $(T, d_p, N_B, \varepsilon I_{SC}, \varepsilon\eta)$ contains useful and redundant information compared to $(T, d_p, N_B, \varepsilon I_{SC})$.

and on page 15, two last paragraph

To assess the degree of redundancy information in different descriptor sets, we employed principal component analysis (PCA), widely used in solving various problems, including identifying defects in solar cells [35]. PCA uses a linear combination of the original variables to construct the new variables (principal component, PC) while keeping maximum variance information. PCs are uncorrelated, and PCA allows one to evaluate each PC's contribution to the total variance of the information. In the case of some particular principal component having a low information variance ratio, it can be discarded with little to no loss of useful information.

PCs were built for different combinations of photovoltaic parameters and solar cell characteristics for the full set of simulated data, and the results are listed in Table 2. As evident, when only changes in short-circuit current are considered along with the solar cell's base parameters and temperature, no excessive information is present (in the case of the descriptor set $(T, d_p, N_B, \varepsilon I_{SC})$, all four principal components exhibit a high ratio of information variance). And vice versa, when estimating $N_{Fe}$ using a maximal set of seven descriptors $(T, d_p, N_B, \varepsilon I_{SC}, \varepsilon\eta, \varepsilon V_{OC}, \varepsilon FF)$ obtained under monochromatic illumination five PCs account for more than 99.5% of the variance in the input data. Therefore, applying PCA to transform the seven input variables and using only five is fully justified, as it significantly simplifies calculations with minimal impact on estimation accuracy. For the same set of descriptors obtained under AM1.5 illumination, the number of really independent variables is six. In general, if the estimation of iron concentration is based on changes in multiple photovoltaic parameters, it is advisable to apply PCA to transform the original data. Thus, the simultaneous use of $\varepsilon\eta$ and $\varepsilon I_{SC}$ practically does not alter the number of independent variables (four) compared to the initial set of descriptors. With the additional use of $\varepsilon V_{OC}$ values obtained under AM1.5 illumination, it is advisable to consider five independent variables. For the same set of descriptors in a monochromatic illumination case, one can limit oneself to using only four independent components (cumulative variance ratio for PC4 and PC5 does not exceed 1.3%).

**Comment 5.** *Your paper discusses the influence of doping levels on the response of solar cells to iron contamination. Author should explain how varying the doping concentration affects the sensitivity of photovoltaic parameters to iron presence through the reference: Augmented photovoltaic performance of Cu/Ce-(Sn: Cd)/n-Si Schottky barrier diode utilizing dual-doped Ce-(Sn: Cd) thin films.*

**Reply:**

The primary reason doping concentration $N_B$ influences the sensitivity of photovoltaic parameters to iron presence is that the $N_B$ determines the Fermi level $E_F$ position. In turn, the rate of Shockley-Read-Hall recombination — and consequently, variations in photovoltaic parameters due to iron impurities — depends on the relative positioning of $E_F$ concerning the $Fe_iB_s$ and $Fe_i$ levels. Additionally, the equilibrium ratio of $Fe_iB_s$ and $Fe_i$ concentrations is also determined by the Fermi level position [28, 29]. Therefore, $N_B$ affects the number of defects that change their state due to the complete dissociation of $Fe_iB_s$ pairs, leading to corresponding relative changes in photovoltaic parameters analyzed in this study. Besides, the $N_B$ concentration also affects the SCR depth (see Fig. 4 in manuscript). The ratio of different charge states for both interstitial iron atoms and iron-boron pairs differs between the SCR and the bulk of the base, leading to distinct SRH recombination rates and variations in photovoltaic conversion efficiency for structures with different doping levels. Furthermore, according to Klaassen's model [23], the concentration of ionized impurities influences charge carrier mobility and, consequently, the diffusion coefficient $D_n$, diffusion length $L_n$, and photoelectric conversion efficiency (see Eqs. (4), (5), and (7) in the manuscript). However, the effect of $N_B$ via $D_n$ and $L_n$ is significantly weaker than its influence through $E_F$ and SCR depth variations. Minor effects are expected as well due to both bandgap narrowing and changes in light absorption by free carriers with varying doping levels. The impact of doping level on photovoltaic parameters has been studied in heterojunction [36], thin-film [37], and perovskite [38] solar cells. Moreover, it has been shown [37] that doping concentration variations affect other barrier structure parameters, such as saturation current and ideality factor.

This answer is incorporated in the text on page 4, paragraph 4, line 1-2. Reference is included in the revised manuscript (references 1)

...while the presence of the acceptor state $Fe_iB_s$ causes the carrier lifetime to be doping-dependent under low injection conditions [FeB:Schmidt].

The relationship between $N_B$ and $E_F$ is the key factor in the influence of doping level on the sensitivity of photovoltaic parameters to iron presence. Specifically, the rate of SRH recombination — and consequently, variations in photovoltaic parameters due to iron impurities — depends on the relative positioning of $E_F$ concerning the $Fe_iB_s$ and $Fe_i$ levels. Additionally, the equilibrium ratio of $Fe_iB_s$ and $Fe_i$ concentrations is also determined by the Fermi level position [FeB:kinetic,MurphyJAP2011]. Therefore, $N_B$ affects the number of defects that change their state due to the complete dissociation of $Fe_iB_s$ pairs, leading to corresponding relative changes in photovoltaic parameters analyzed in this study. Besides, the $N_B$ concentration also affects the SCR depth (see Fig. 4). The ratio of different charge states for both interstitial iron atoms and iron-boron pairs differs between the SCR and the bulk of the base, leading to distinct SRH recombination rates and variations in photovoltaic conversion efficiency for structures with different doping levels. Furthermore, according to Klaassen's model [KLAASSEN953], the concentration of ionized impurities influences charge carrier mobility and, consequently, the diffusion coefficient $D_n$, diffusion length $L_n$, and photoelectric conversion efficiency (see Eq. (4)). However, the effect of $N_B$ via $D_n$ and $L_n$ is significantly weaker than its influence through $E_F$ and SCR depth variations. Minor effects are expected as well due to both bandgap narrowing and changes in light absorption by free carriers with varying doping levels. The impact of doping level on photovoltaic parameters has been studied in heterojunction [8], thin-film [10], and perovskite [6] solar cells. Moreover, it has been shown [10] that doping concentration variations affect other barrier structure parameters, such as saturation current and ideality factor.

**Comment 6.** *In your findings, Author mentions that changes in short-circuit current under monochromatic illumination are the most reliable for estimating iron concentration. An author should provide more details on the methodology used to derive this conclusion and any potential limitations of this approach?*

**Reply:**

We employed two key metrics to identify the solar cell parameter whose changes, resulting from the $Fe_iB_{Si} \rightleftarrows Fe_i + B_{Si}$ reconstruction, enable the most reliable determination of iron concentration. Specifically, these metrics are: (1) the monotonicity of the relative change in the parameter value as a function of impurity concentration, which is a necessary condition for the unambiguous estimation of $N_{Fe}$; and (2) the absolute magnitude of the parameter change, which allows for more precise measurements and, consequently, a more accurate estimation of $N_{Fe}$. The first criterion is not satisfied by $\varepsilon FF$, $\varepsilon V_{OC}$, and $\varepsilon \eta$ (the latter two under AM1.5 illumination). At the same iron concentration, $\varepsilon I_{SC}$ values under monochromatic illumination exceed those under AM1.5 illumination. As mentioned earlier, this effect deals with differences in the generation locations of non-equilibrium carriers under different lighting conditions. Additionally, under identical conditions, the changes in open-circuit voltage are significantly weaker than those in short-circuit current or efficiency. Since $\varepsilon I_{SC}$ and $\varepsilon \eta$ are of the same order, it is advisable to select the more reliable parameter using additional metrics. Notably, short-circuit current determination, unlike efficiency, does not require additional calculations and can be directly extracted from the raw measured $I$-$V$ curves. Furthermore, $\varepsilon I_{SC}$ is virtually independent of illumination intensity (whereas $\varepsilon \eta$ exhibits a weak dependence), leading to two key advantages: (a) iron concentration can be determined using an uncalibrated for-intensity monochromatic light source; (b) the influence of shading caused by electrodes, along with the antireflective and passivating layers of the solar cell, is reduced.

Thus, short-circuit current is the most suitable parameter for estimating the concentration of iron impurities, as its changes during the $Fe_iB_{Si} \rightleftarrows Fe_i + B_{Si}$ transformation can be effectively utilized. Determining photovoltaic parameters under monochromatic illumination, with a wavelength corresponding to the predominant absorption in the solar cell base, is more effective than using AM1.5 illumination. The most viable alternatives are solar cell efficiency and open-circuit voltage; however, their applicability is limited at low base doping levels ($< 10^{16}$ cm$^{-3}$) due to non-monotonic variations in response to increasing iron concentration. In our view, using the fill factor for iron concentration estimation is impractical. These conclusions are validated by experimental results, which show that short-circuit current provides the most accurate determination of iron concentration.

The limitations of the proposed method may arise from the presence of a significant number of recombination-active defects unrelated to iron, as well as high series resistance (which distorts the short-circuit current) and/or shunt resistance (which primarily affects the open-circuit voltage).

The Conclusion has been revised according to the Reviewer's advice — see page 17, 1st and 2nd paragraph

The feasibility of using relative changes in short-circuit current, open-circuit voltage, fill factor, and efficiency resulting from the dissociation of FeB pairs to estimate the concentration of iron impurities in a solar cell has been analyzed. Two key metrics were used to identify the solar cell parameter whose changes, resulting from the $Fe_iB_{Si} \rightleftarrows Fe_i + B_{Si}$ reconstruction, enable the most reliable determination of iron concentration. Specifically, these metrics are: (1) the monotonicity of the relative change in the parameter value as a function of impurity concentration, which is a necessary condition for the unambiguous estimation of $N_{Fe}$; and (2) the absolute magnitude of the parameter change, which allows for more precise measurements and, consequently, a more accurate estimation of $N_{Fe}$. The first criterion is not satisfied by $\varepsilon FF$, $\varepsilon V_{OC}$, and $\varepsilon \eta$ (the latter two under AM1.5 illumination). At the same iron concentration, $\varepsilon I_{SC}$ values under monochromatic illumination exceed those under AM1.5 illumination. As mentioned earlier, this effect deals with differences in the generation locations of non-equilibrium carriers under different lighting conditions. Additionally, under identical conditions, the changes in open-circuit voltage are significantly weaker than those in short-circuit current or efficiency. Since $\varepsilon I_{SC}$ and $\varepsilon \eta$ are of the same order, it is advisable to select the more reliable parameter using additional metrics. Notably, short-circuit current determination, unlike efficiency, does not require additional calculations and can be directly extracted from the raw measured $I$-$V$ curves. Furthermore, $\varepsilon I_{SC}$ is virtually independent of illumination intensity (whereas $\varepsilon \eta$ exhibits a weak dependence), leading to two key advantages: (a) iron concentration can be determined using an uncalibrated for-intensity monochromatic light source; (b) the influence of shading caused by electrodes, along with the antireflective and passivating layers of the solar cell, is reduced.

Thus, short-circuit current is the most suitable parameter for estimating the concentration of iron impurities, as its changes during the $Fe_iB_{Si} \rightleftarrows Fe_i + B_{Si}$ transformation can be effectively utilized. Determining photovoltaic parameters under monochromatic illumination, with a wavelength corresponding to the predominant absorption in the solar cell base, is more effective than using AM1.5 illumination. The most viable alternatives are solar cell efficiency and open-circuit voltage; however, their applicability is limited at low base doping levels ($< 10^{16}$ cm$^{-3}$) due to non-monotonic variations in response to increasing iron concentration. In our view, using the fill factor for iron concentration estimation is impractical. These conclusions are validated by experimental results, which show that short-circuit current provides the most accurate determination of iron concentration.

**Comment 7.** *An Author must improve the introduction section in the application part through the recent referencs CuO-La2O3 Composite-Enabled MIS Schottky Barrier Diodes: A Novel Approach to Optoelectronic Device Diversification; Enhancing photovoltaic applications through precipitating agents in ITO/CIS/CeO2/Al heterojunction solar cell; Manifestation on the choice of a suitable combination of MIS for proficient Schottky diodes for optoelectronics applications: A comprehensive review.*

**Reply:**

We sincerely thank the Reviewer for suggesting the inclusion of recent references (cited as References 2, 3, and 9 in the revised manuscript). Below, we present an improved version of the 1st paragraph of Introduction.

The necessity for renewable energy sources to meet the growing global demand for sustainable and environmentally friendly energy alternatives has become evident. Among the wide range of renewable energy sources, sunlight is the cleanest, safest, and most abundant source for use in sustainable energy to support economic growth [1]. The utilization of solar energy heavily depends on the use of photovoltaic cells. The development of next-generation solar cells is primarily driven by the search for novel materials suitable for their fabrication. Particular attention is given to exploring the potential use of composites and nanoparticles (e.g., Cu-La-based systems [2], cerium oxide, and copper indium sulfate [3]), MAX phases [4,5], and chalcogenides (such as GeSe, $MoSe_2$, $Sb_2Se_3$, and SnSe as hole transport materials [6] or $SnS_2$ and $WS_2$ as electron transport materials [7]), as well as metal silicides (e.g., $FeSi_2$ as an absorber layer [8]). These studies cover a broad range of materials [9], with the primary goal of developing highly efficient and cost-effective photovoltaic devices. Frequently, these novel materials are integrated with silicon in solar cells [8,10]. However, it is worth noting that traditional silicon-based devices continue to play a dominant role in the photovoltaic market [11,12].

**Response to Reviewer #2**

**Comment 1.** *The abstract section should be more informative.*
**Reply:**
**Comment 2.** *The novelty of the work is missing in the introduction. Authors should explain what are the key advantages of iron's impact on silicon solar cell?*
**Reply:**
**Comment 3.** *Authors should improve the image quality of all figures.*
**Reply:**
**Comment 4.** *Author should explain how does the band alignment affect the overall performance of the solar cell?*
**Reply:**
**Comment 5.** *What are the primary sources of iron contamination in silicon used for solar cells?*
**Reply:**
**Comment 6.** *What role do recombination centers created by iron play in the modeling of solar cell performance?*
**Reply:**
**Comment 7.** *Author should discuss and cited recent Si based solar cell in the revised manuscript: DOI : $10.1016/j.mseb.2024.117360$, $DOI : 10.1016/j.mseb.2023.117141$, $DOI : 10.1016/j.mseb.2024.117817$, $DOI : 10.1007/s42247 - 024 - 00821 - y$, $DOI : 10.1016/j.inoche.2024.112785$*
**Reply:**
   We sincerely appreciate the reviewer's valuable suggestion. Most of the recommended works are highly relevant, and we have cited them in multiple sections of the manuscript. Advised articles are referenced as References 8, 4, 6, 7, and 5 in the revised version.

   So, we discuss and cited suggested papers in the Introduction, first paragraph

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The necessity for renewable energy sources to meet the growing global demand for sustainable and environmentally friendly energy alternatives has become evident. Among the wide range of renewable energy sources, sunlight is the cleanest, safest, and most abundant source for use in sustainable energy to support economic growth [1]. The utilization of solar energy heavily depends on the use of photovoltaic cells. The development of next-generation solar cells is primarily driven by the search for novel materials suitable for their fabrication. Particular attention is given to exploring the potential use of composites and nanoparticles (e.g., Cu-La-based systems [2], cerium oxide, and copper indium sulfate [3]), MAX phases [4,5], and chalcogenides (such as GeSe, $MoSe_2$, $Sb_2Se_3$, and SnSe as hole transport materials [6] or $SnS_2$ and $WS_2$ as electron transport materials [7]), as well as metal silicides (e.g., $FeSi_2$ as an absorber layer [8])

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Despite its one-dimensional modeling approach, SCAPS is extensively used for modeling various types of solar cells [6,7,8,Joshi2024,Ravidas2024,Liu2024,You2023] in general and for investigating the effects of defects on their performance [6,8,AitAbdelkadir2023,Liang2024,SCAPSDefect3] in particular.

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on page 4, last paragraph

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Impact of change of iron defects was investigated as a function of temperature from 290 K to 340 K, base depth from 180 $\mu m$ to 380 $\mu m$, base doping level from $10^{15}$ cm$^{-3}$ to $10^{17}$ cm$^{-3}$, and total impurity iron atom concentration from $10^{10}$ cm$^{-3}$ to $10^{14}$ cm$^{-3}$. It is worth noting that investigating the effects of doping density, defect density, temperature, and active layer thickness on photovoltaic parameters is a well-established practice [6,7,8]. For each illumination scenario, calculations were carried out with 11 different temperature values and 5 base depth values, evenly distributed within the specified ranges.

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However, the effect of $N_B$ via $D_n$ and $L_n$ is significantly weaker than its influence through $E_F$ and SCR depth variations. Minor effects are expected as well due to both bandgap narrowing and changes in light absorption by free carriers with varying doping levels. The impact of doping level on photovoltaic parameters has been studied

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in heterojunction [8], thin-film [10], and perovskite [6] solar cells. Moreover, it has been shown [10] that doping concentration variations affect other barrier structure parameters, such as saturation current and ideality factor.

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- At low boron concentrations ($N_B < 10^{16}$ cm$^{-3}$), the dependence of $\varepsilon FF$ on $N_{Fe}$ is notably non-linear. Within the used concentration range, two regions of decrease and two regions of increase in $\varepsilon FF$ are observed. A similar relationship between the fill factor and defect concentration was observed in BaZrSe$_3$–based perovskite solar cells [6];

**Comment 8.** *How does the modeling in this study contribute to the design of processes for impurity control in silicon?*
**Reply:**
**Comment 9.** *State the main findings in the conclusions.*
**Reply:**

# References

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