Dear Editor and Reviewers,

We sincerely thank you for taking the time to review our manuscript "Extracting the iron concentration in silicon solar cells using photovoltaic parameters and machine learning" (Ms. Ref. No.: SEJ-D-25-01089). 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. The location of revisions is pointed by red color and highlighted in yellow in "MarkedManuscript.pdf". 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 Solar Energy.

Response to Reviewer #1

Comment 1. *The introduction lacks the role of iron valency (ferrous or ferric) in silicon solar cells.*

Reply:

Reviewer is correct that ferrous (Fe^{2+}) and ferric (Fe^{3+}) states deserve consideration, as they are the most common and stable charge states of iron. These ionic forms typically occur in compounds where iron forms chemical bonds (either ionic or covalent) with other elements, as well as in cases where iron is present as an impurity in solid materials. In silicon, iron can also exist in a trivalent (ferric) state when it substitutes for a silicon atom at a lattice site. However, under normal conditions, the concentration of substitutional iron is extremely low, less than 1% of the total iron impurity atoms [1]. Increasing the concentration of substitutional iron requires special sample processing, such as high-temperature annealing or irradiation. Moreover, substitutional iron acts as a weak recombination center, so its influence on the properties of silicon solar cells can be neglected. The ferrous form is virtually absent in silicon. The majority of iron impurity atoms in silicon occupy positions, where they can exist in either a neutral (Fe_i^0) or positively charged (Fe_i^+) state, depending on the position of the Fermi level [2]. In *n*-type silicon, Fe_i is more likely to exist in a neutral state, whereas in *p*-type silicon, it is more likely to be positively charged. Even when interstitial iron forms complex point defects, such as iron–boron pairs (Fe_iB_s), no valence bonds are formed. In interstitial configuration, iron acts as an active recombination center.

Consequently, in silicon solar cells, the role of iron valence is negligible, in contrast to other types of solar cells, such as perovskite solar cells [3]. Specifically, in $MAPbI_3$-based devices, both Fe^{3+} and Fe^{2+} point defects are observed, with Fe^{3+} being electronically inactive in terms of recombination.

We have added the relevant information to the Introduction (page 2, third paragraph from the top)

> (ii) iron is one of the most prevalent, ubiquitous, and efficiency-limiting metallic impurities [4, 5].
>
> It is well known that ferrous (Fe^{2+}) and ferric (Fe^{3+}) are the most common and stable charge states of iron in most materials. But the majority of iron impurity atoms in silicon occupy interstitial positions, where they can exist in either a neutral (Fe_i^0) or positively charged (Fe_i^+) state, depending on the position of the Fermi level [6, 2]. In *n*-type silicon, Fe_i is more likely to exist in a neutral state, whereas in *p*-type silicon, it is more likely to be positively charged. Even when interstitial iron forms complex point defects no valence bonds are formed. In silicon, iron can also exist in a trivalent (ferric) state when it substitutes for a silicon atom at a lattice site. However, under normal conditions, the concentration of substitutional iron is extremely low, less than 1% of the total iron impurity atoms [1]. The ferrous form is virtually absent in silicon. Consequently, in silicon solar cells, the role of iron valence is negligible, in contrast to other photovoltaic technologies, such as perovskite-based devices [3].
>
> It is well established that in *p*-type material, iron tends to bind with dopant atoms such as boron,

Comment 2. *The work didn't deal with the redox reaction of iron in silicon solar cells.*

Reply:

In the context of crystalline silicon, iron does not participate in classical redox (reduction-oxidation) reactions as it does in aqueous solutions or oxide matrices. In such environments, iron can exist in distinct chemical valence states (e.g., Fe^{2+}/Fe^{3+}), and redox reactions involve the transfer of electrons between these states.

In silicon, however, iron atoms are incorporated as isolated point defects (Fe_i) or as complexes with boron (Fe_iB_s). Their charge states (e.g., Fe_i^0, Fe_i^+) are determined by the position of the Fermi level and the local electronic environment within the silicon lattice-not by chemical oxidation or reduction processes [**?**].

The transitions between different charge states of iron-related defects in silicon are governed by electronic capture and emission processes (i.e., the exchange of electrons or holes with the conduction or valence band), rather than by redox reactions in the chemical sense.

These processes are described within the framework of semiconductor defect physics, specifically through Shockley-Read-Hall recombination theory, and are crucial to understanding the recombination activity of Fe_i and Fe_iB_s in silicon.

The dominant factor affecting solar cell performance is the recombination activity of iron-related point defects, which act as deep-level traps for charge carriers. The kinetics of Fe_i and Fe_iB_s formation, dissociation, and charge-state transitions are well understood in terms of defect energetics and do not involve classical redox chemistry.

References

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