# Scientific Review Report

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# Peer Reviewer's Comments

## Note from the Peer Reviewer, Jane Doe

Dear author,

My name is Dr. Jane Doe, and it has been a pleasure reviewing your manuscript. I have a PhD in materials science and engineering, and my areas of expertise include nanomaterials for energy and environmental applications. I have 6 years of peer review experience, and I have reviewed for Materials and Design (IF: 7.991), Scripta Materialia (IF: 5.611), and ACS Applied Materials & Interfaces (IF: 9.299) among others.

I have carefully read and evaluated your manuscript and provided suggestions to strengthen the presentation of your research and highlight its relevance and originality. This report also includes comments on the manuscript's language, structure, and submission readiness from the Senior Science Editor and Managing Editor that I hope you will find useful.

I wish you the very best with the submission of your manuscript!

## Summary

- Is the paper ready for submission in its current form?
  No

- Major issues – Likely to cause journal rejection

  The low-cost HIT solar cells prepared in this study seem to have significant application prospects and are therefore expected to draw attention from researchers working in this field. However, the manuscript requires significant improvements. The research rationale must be clearly stated at the beginning of the abstract. The introduction, experimental section, results, and conclusions have substantial scope of improvement. Further addition of data and background information will help in improving the manuscript significantly by presenting a holistic picture of the system developed in this study.

  - The manuscript lacks a novelty statement. Metallurgical Si has been already used for the fabrication of solar cells, and HIT solar cells have been previously studied by AFORS-HET. Perhaps, this study attempts to combine metallurgical Si and HIT solar cells. However, the novelty of this aspect must be clearly highlighted. For example, this is perhaps the first study in which metallurgical Si is used for AFORS-HET. This must be stated clearly.
  - With regard to the above point, it is also necessary to clearly explain the features/specialties of HIT solar cells. It would be ideal if a section on the description of HIT solar cells and how they are different from other solar cells is included in the introduction.

- What is meant by "significant," with respect to the results of the previously reported AFORS-HET simulations?
- The compensation effect, which plays a crucial role in the cells, must be discussed in the introduction.
- What was the thickness of each Si layer in the fabricated HIT cells? This is a crucial aspect in fabrication. Also, please indicate "contact" in the schematic of the HIT solar cells.
- The schematic (Figure 1) indicates a p+-type layer, while the simulated defect state distribution graph mentions a p-type layer (Figure 2a). Please clarify this discrepancy.
- In Table 2, it is listed that $\eta$ of the HIT solar cell with metallurgical Si increased up to 21.17% when the B concentration was zero. Was the same ensured experimentally too? If so, how?
- How would the cell properties be affected if only Cu impurities are present?
- How would the cell properties be affected if Cu impurity is fixed and Fe impurities are varied? These data are important to present a holistic picture of the material properties.
- It is quite clear that the cell properties are not affected much by the compensation effect. What do you think is the plausible reason for this?
- The simulated temperature coefficient (TC) of the photoelectric conversion efficiency was lower than the measured value. What do you think could be a plausible reason for this? Investigating the effect of temperature on the I–V characteristics may shed light in this regard.

- Minor issues – Likely to cause delays in journal acceptance

There are a few places in the manuscript where some essential details are missing. See the points below.

- Experimental details for the measurement of resistivity, minority-carrier life time, and metal impurities must be provided.
- Details on acid etching of the substrate must be provided.
- Various methods have been listed for the purification of Si by metallurgical methods. Which method was used in this study? Please explain this clearly.
- For the graph shown in Figure 4, what was the P concentration?
- Overall, the results section must be more detailed. For example, details on the experimental investigation and analysis of the material properties must be provided in more detail to allow better comprehension of the system studied.

- Does the paper present novel ideas/a novel direction with regard to the field of research?

The paper does seem to present a novel idea. However, the novelty statement is missing in the manuscript. Please go through my previous recommendations to address these points.

- Is the research rationale sound? (is the reason for conducting the research explained clearly in the paper?)

The research rationale is sound, and the reason for conducting the research is present in the paper. However, it might be stated more boldly. E.g., "To render the HIT solar cell fabrication process more economical, we attempted to integrate metallurgical Si with HIT solar cells...."

- Does the journal accept this article type?

  The current manuscript is a complete research article, and this type of manuscript is accepted by the target journal.

- Does the research in this article lie within the target journal's scope?

  ACS Applied Materials and Interfaces publishes works related to the development and application of materials. The current study on the effect of material properties on the solar cell performance fits well into the scope of the journal.

- Does the paper present novel ideas or build on the research published in the target journal?

  The target journal publishes papers related to materials that can improve the efficiencies of solar cell. The current study presents an analysis of the material composition (metallurgical Si) that ultimately aids in improving the solar cell performance. Hence, the paper builds on the research published in the target journal.

# Assessment by paper section

## Title and Abstract

- Are the Title and Abstract representative of the study? How can they be made more compelling?

  The title of the manuscript is well in line with the manuscript content. The abstract contains most of the essential information. However, the research rationale must be clearly stated at the beginning of the abstract.

- Can a wide readership understand the Title and Abstract independent of the main text? Can they be made more accessible to readers across disciplines?

  Given the rather specialized area of study, the title and abstract may be a little difficult for a wide readership to follow. I believe adding the rationale at the start of the abstract, as suggested above, may partly remedy this issue. I also recommend talking about the wider implications of your findings, as this may help general readers to understand what your study's findings mean for the field.

## Introduction

- Is the literature review complete and which other papers can the author cite?

  The literature review must be more exhaustive. Most importantly, when results of AFORS-HET simulations are being published, the following reference should be cited:

**Varache, R., Leendertz, C., Gueunier-Farret, M.E., Haschke, J., Muñoz, D. and Korte, L., 2015. Investigation of selective junctions using a newly developed tunnel current model for solar cell applications. *Solar Energy Materials and Solar Cells*, *141*, pp. 14-23.**

More references corresponding to the description of HIT solar cells and compensation effect must be included. Following are some examples:

- **Zhao, L., Zhou, C.L., Li, H.L., Diao, H.W. and Wang, W.J., 2008. Design optimization of bifacial HIT solar cells on p-type silicon substrates by simulation. *Solar Energy Materials and Solar Cells*, *92*(6), pp. 673-681.**
- **Froitzheim, A., Stangl, R., Elstner, L., Kriegel, M. and Fuhs, W., 2003, May. AFORS-HET: a computer-program for the simulation of heterojunction solar cells to be distributed for public use. In *3rd World Conference on Photovoltaic Energy Conversion, 2003. Proceedings of* (Vol. 1, pp. 279-282). IEEE.**
- **Dwivedi, N., Kumar, S., Bisht, A., Patel, K. and Sudhakar, S., 2013. Simulation approach for optimization of device structure and thickness of HIT solar cells to achieve~ 27% efficiency. *Solar energy*, *88*, pp. 31-41.**

- Are the study objectives clearly stated and do they align with the methods and results?

  The study objective is clearly outlined in the introduction, and it is in line with the methods and results of the study. However, I recommend clarifying the key motivation for the study. You have stated that AFORS-HET simulation has already been employed in the investigation of HIT solar cells. If so, why would the current study be necessary? Please clarify this point.

## Methods

- Is the research design appropriate? What are the gaps, and what should be done to fill the gaps?

  The research design can be improved. Basically, the impurity effects and concentration effects are being investigated, both experimentally and by simulation. Ideally, a systematic approach should be adopted. For instance, only Fe and Cu impurities are considered. Thus, one must first examine the effect of the individual impurities (i.e., only Cu and only Fe). Going forward, each impurity must be fixed while the other is varied. Similarly, for the compensation effect, B and P should be examined individually as well as in combination.

- Is the research methodology sound and relevant to the field? Are the methods detailed enough to be reproduced by a skilled researcher?

  The research methodology (AFORS-HET simulation, PEVCD, etc.) is sound and is widely used in the field of solar cells. The methods include sufficient details regarding the instruments and equipment employed in the study. However, details on GDMS must be added in this section.

- Has the manuscript been prepared in accordance with the EQUATOR Network's research reporting guidelines? What are the gaps, and what should be done to fill the gaps?

  The EQUATOR Network's research reporting guidelines are not applicable to this field of study.

## Results and Discussion

- Does the data appear accurate, and has it been interpreted appropriately? Flag cases of insufficient or insignificant data with the author.

  The data are accurate and have been interpreted accurately. However, at several instances, further experimental data are required to explain the underlying mechanism behind the improved conversion efficiency. Please go through my recommendations in the manuscript and above points for the same.

- Do the tables and figures clearly present the data, and do they align with the description of key results in the text? Flag inconsistencies and inaccuracies with the author.

  The figures and tables do a good job of presenting the data. They align with the discussion of the key results as well. A few inconsistencies and minor issues have been noted. For instance, in Figure 1, you have specified p+-type layer, whereas the main text says p-type layer. Please consider elaborating on this. Also, in Figure 4, please specify the P concentration.

- Should the author get their data verified by a statistician or submit analyzed datasets to the journal?

  The data analysis is sound and need not be verified by a statistician.

- Are the research implications clearly mentioned? If they are mentioned, are they sound? If they are not mentioned, what tips should the author follow?

  The research implication is mentioned very clearly. It is stated that a small amount of impurity does not affect the cell performance; moreover, despite the poorer material properties, HIT solar cells fabricated with metallurgical Si have a significant potential in large-scale industrial manufacturing.

- Are the concluding statements clear, and do they mention the contributions, limitations, and next steps for other researchers in the field?

  The manuscript has a concluding section that mentions the overall conclusion of the study. The numerical values of the cell parameters are also reported in this section. However, the limitations of the study are not stated. A statement on the future prospects of this study or how this study can be utilized by other researchers is missing. Most importantly, a comparison of the conversion efficiency of this cell with the other cells must be present in order to the highlight the competitive efficiency of these cells.

# Senior Science Editor's Comments on Language and Paper Structure

- How was the paper's overall language quality prior to editing?

  Although the language was comprehensible, several changes were required throughout the document to polish the language for accuracy, grammar, and a native tone. I have discussed the same and provided examples in the next point for clarity.

- What were the top 3 recurring grammar and language issues found and edited for native tone?

  - Sentence construction to introduce formality: The intended meaning was not reflected very clearly in some sentences. E.g., "The Si substrate used in this simulation was 170 $\mu$m which is smaller than 190 $\mu$m of bare Si wafer due to the thickness reduction by acid etching," can be better written as "Owing to the reduction in thickness upon acid etching, the Si substrate (170 $\mu$m) used in this simulation was smaller than the bare Si wafer (190 $\mu$m)."
  - Wordiness: The use of too many words to convey one idea can muddle the message and divert the reader's attention. Therefore, in writing, especially academic writing, ideas need to be conveyed as concisely as possible. One way of doing this is to use concise alternatives to phrases. E.g., "energy levels of Fe and Cu in Si" can be more concisely written as "Fe and Cu energy levels in Si"
  - Technical accuracy: A range already denotes an approximate value. Hence, the use of the approximation symbol ("~") in between the values is incorrect. For e.g., the actual form is 5–10 nm (with an en dash (–) in between, not a hyphen (-)) and not 5 ~ 10 nm.

- Does the edited paper adhere to the target journal's language preference?

  The journal guidelines do not state specifically about the use of American or British English. However, the manuscript has been edited in American English as per the instructions.

- What types of changes were made for improvements to paper flow and how has the paper's readability improved because of these?

  Comments have been added at relevant places to fill in the missing gaps/ideas.

  - The abstract was revised provide a concise summary of the study to the readership.
  - Table 1 has been moved before Results and Discussion because tables and figures should be present close to their first mention in the main text.
  - Detailed suggestions have been made to enhance the flow of the results and discussion section, which currently lacks an experimental investigation and analysis of the material properties.

## Senior Science Editor's and Managing Editor's Comments on the Paper's Journal Readiness

- What details or documents are missing in the paper submission package based on the target journal's formatting and submission requirements?
    - ♦ A separate cover letter is required for submission, and this has been prepared.
    - ♦ The author names, affiliations, and details on supporting information must be added in the manuscript.

- List out the journal's author preferences and formatting instructions (including the right file formats) that could not be followed and why.

  All the formatting guidelines have been adhered to. The manuscript is inserted into the journal template and is in the .docx format. The references have not been formatted as they were excluded from the edit.

- Does the target journal have a word count limit, and does the paper adhere to this limit after editing?

  There is a word count limit for the abstract (maximum 300 words), and your abstract adheres to this word limit. However, there is no word limit for the manuscript as a whole.

- Does the paper need to be split for submission?

  This is a relatively short paper, and the ideas/results/conclusion are present in a concise manner. It need not be split for submission.

- Does the paper need to be blinded for review, and has it been blinded?

  There are no results that are contradictory to previous studies. The paper need not be blinded for review.

- Have ethical and financial declarations been provided? If not, alert the author to do so and explain why.

  Financial declarations have been provided. No human or animal studies were conducted.

- Is a conflict-of-interest statement provided? If not, alert the author to do so and explain why.

  A conflict of interest statement has been provided.

- Has a data availability statement been provided? If not, alert the author to do so and explain why.

  The data availability statement has not been provided. This has been indicated in the manuscript as a comment (the section on supporting information).

- Has the corresponding author been identified for journal interaction?

  The author names and affiliations have not been provided.

- Are all the references, tables, and figures present?

  The references were not checked as they were excluded from editing. All the tables and figures are present.

- Are the references in the right format and the figures and tables labelled appropriately?

  The references were not checked as they were excluded from editing; however, the in-text citations are in the correct format.