Paper topic: **Density functional theory study of copper zinc tin sulphide (Cu_2ZnSnS_4) doped with calcium and barium.**

Paper ID: 32

A report of comments from reviewers (in bold) and corrections made (light text) on the SAIP 2019 proceedings paper – rebuttal

Referee 1

Comments

Please find my recommendation and comments for the manuscript.
The manuscript is well written however the following comments should be addressed; however I recommend that the manuscript should be accepted.
The significance of some of the statements and findings in the manuscript is lost, since the author didn't offer a thorough description. Please make sure that the relevance of all terms (more instance kesterite) are described, before using the term in the results and discussion section of the manuscript.
Here are more specific comments:

1. **The following statement was made in the Abstract: "A new doping mechanism was used to dope the structure with the alkali earth metals, Calcium (Ca) and Barium (Ba)." Please explain the statement within the manuscript.**

A description of the procedure used in the study was added to the manuscript, the statement was rephrased. We used adsorption locator module from material studio to perform the adsorption on the surface of the structure. We say new because it has not been used for related studies and it is combining two modules (CASTEP for calculations and Adsorption locator for adsorption purposes)

2. **Please explain the significance of the following information given towards the end of the Introduction:**
"In the absence of light, a very small amount of atoms is excited and move across the junction. This causes a small voltage drop across the junction. In the presence of light, more atoms are excited and flow through the junction and cause a large current at the output." Please state, within the manuscript, how it ties into the body of work (findings) presented.

This statement was removed and replaced with the following sentence to conclude the introduction: This study seeks to investigate photovoltaic properties of CZTS material using computer modelling techniques for application in solar cells. The statement did not connect properly with the paragraph.

3. **The author states on more than one occasion in the results in discussion that the CZTS are kesterite type. Note that no explanation was given to clarify what the significance of a kesterite type CZTS is. It is suggested that a small description should be added to the Introduction.**

A short description of kesterite type of material was added in the manuscript**:** Kesterite is a sulphide mineral with a formula $Cu_2(Zn,Fe)SnS_4$.

4. **A more complete discussion should be given as to way the absorption coefficient of the Ba-doped CZTS material. This following sentence is insufficient and offers no real explanation for the findings: "These peaks can be credited to the position of the elements in the periodic table and their photo electrolytic properties." Please explain why the position of the elements in the**

periodic table is relevant, and how the photo-electrolytic properties of the Ba-doped CZTS material are different from the Na- and Ca-doped CZTS materials.

The statement **"**these peaks can be credited to the position of the elements in the periodic table and their photo electrolytic properties**"** is included to indicate that the position of elements in the periodic table was considered with photo-electrolytic properties of that element that comes with being in that specific position. Since we are doping with alkali earth metals, calcium comes before barium so we expected it to have more electrons than calcium hence it responds better when exposed to light. However this statement could be removed and it will not change the intended message of the paper.

5. **In the introduction and conclusion the author states that:**
"CZTS film shows a tetragonal structure with preferential orientation along the (1 1 2) plane."
Please elaborate as to why this is the preferred plane.

CZTS 112 surface is the dominant and stable plane as observed mostly from experimental works on the synthesising of such material, it satisfies most of the adsorption conditions. This suggested that altering this plane could bring about great changes to the morphology of the structure and thus bring observable changes, hopefully improvements on properties being studied.

Referee 2

Comments

1**. Please address reviewer comments.**

Reviewer comments were addressed accordingly.

2. **Please ensure manuscript is formatted according to SAIP Conference Proceedings layout style. (Guidelines and Templates link on Indico)**

The paper was typed using the SAIP template downloaded from the website.

3. **Deadline: 1 June 2020.**
A corrected version of the proceedings was uploaded before date.

Referee 3

Comments

Your revised manuscript has been received, thank you. Please submit a detailed rebuttal, responding to reviewer comments.
This can be uploaded on Indico or e-mailed directly to me.
The deadline for this 12h00 on 22 June 2020.
Please confirm receipt of this communication by e-mailing me directly.
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