

Reviewers Report ID 56

The paper titled “**Thermoelectric properties of CdGa₂O₄ spinel**” is an interesting paper investigating the thermoelectric property of the CdGa₂O₄ via VASP simulation. Prior to the publication or acceptance of this manuscript, the author/s must incorporate (the following suggestions) and address the following comments:

Abstract

1. What is ZT? Define it in the first use.

Response: Defined.

Introduction

2. “Although a number of materials have been studied ...”. The author must at least give an example/s of those materials that have been previously studied with valid references.

Response: Several examples and references provided.

3. “Generally, a spinel is a hard glassy mineral that occur as octahedral crystals ...”. This sentence is misleading as spinel’s are known to consist of both the octahedral and tetrahedral sites occupied by atoms.

Response : Corrected.

4. “CdGa₂O₄ occurs in an fcc structure of space group Fd3m consisting of 8 formula units”. This sentence seems to be incomplete to me.

Response: Expanded.

5. What is the novelty of the current study? The last paragraph in each paper or article is/must discussing or give the detailed novelty statement of the current study and I am failing to see that in this paper.

Response : Novelty statement provided.

Results and discussion

3.1 Structural and energetic properties

6. Lack of references in a text. For an example, the reference must be given on the last sentence.

Response : Reference provided.

7. Suggestion: start mentioning or calling your tables in a text before presenting it.

Response : Corrected.

3.3 Dynamical and electronic properties

8. The author/s did not say anything about the band gap they have obtained in their results?

Response: Explained and compared to previous DFT study.

3.4 Transport properties

9. First sentence below figure 5 and 6: the author must be clear on which figure they are referring to?

Response : Clarified.

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10. Science – does it make a contribution

Final comment: Well written manuscript. Contribution to science/ Physics community made clear.

11. Grammar

Some proposed corrections to grammar:

- Pg. 1 line 4 in Abstract – “is given by” instead of “is captured in” **Corrected.**
- Pg. 1 line 4/5 in Abstract – “figure-of-merit (ZT)” rather than “figure of merit, ZT,” **Corrected.**
- Pg. 1 last line in Abstract – “From the determined ZT values, we find that...” **Corrected.**
- Pg. 2 line 5 in Methodology – “namely:” **Corrected.**
- Pg. 2 line 9 in Methodology – “applied” instead of “enforced” **Corrected.**
- Pg. 2 line 4 in Methodology – “studies” instead of “study” **Corrected.**
- Pg. 2 – capitalize “Table” when refer in text **Corrected.**
- Pg. 4 4th line from bottom of page – remove “that” **Removed.**
- Pg. 4 last line – use e.g. “shown” or “substantiated” instead of “reinforced” **Corrected.**
- Pg. 6 lines 2 – 5 in Summary – very long sentence – see if cannot perhaps split into 2 shorter sentences. **Corrected.**
- Check consistency in font size of axes on figures. **Corrected.**

Final comment: Overall good grammar- minor punctuation and grammar revisions required.