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Jury Member Report – Doctor of Philosophy thesis.

Name of Candidate: Tao Fan

PhD Program: Materials Science and Engineering

Title of Thesis: First-principles study of advanced thermoelectric materials: methodology and application

Supervisor: Professor Artem Oganov

Name of the Reviewer: Sergey Levchenko

I confirm the absence of any conflict of interest	
	Date: 15-08-2022

The purpose of this report is to obtain an independent review from the members of PhD defense Jury before the thesis defense. The members of PhD defense Jury are asked to submit signed copy of the report at least 30 days prior the thesis defense. The Reviewers are asked to bring a copy of the completed report to the thesis defense and to discuss the contents of each report with each other before the thesis defense.
If the reviewers have any queries about the thesis which they wish to raise in advance, please contact the Chair of the Jury.
Reviewer's Report
• Brief evaluation of the thesis quality and overall structure of the dissertation.
The thesis by Tao Fan on the topic " First-Principles Study of Advanced Thermoelectric Materials: Methodology and Application" is of excellent quality. It includes methodology development and its high-throughput applications. The English writing is very good, and the structure is clear.
• The relevance of the topic of dissertation work to its actual content
The topic of the thesis directly reflects its content.
• The relevance of the methods used in the dissertation
The thesis includes method development specifically for the given application (thermoelectric materials). All employed approximations are carefully tested and are shown to provide a good balance between accuracy and computational cost.

- The scientific significance of the results obtained and their compliance with the international level and current state of the art

The methodology developed as part of the thesis work was implemented in a publicly available program package. It not only conveniently combines existing methods in one package, but also improves them, going beyond state of the art in the field. Moreover, the package includes tools for automation for high-throughput calculations based on the state-of-the-art automation software, which makes it even more attractive.

- The relevance of the obtained results to applications (if applicable)

Using the newly developed methodology, the author predicts several very promising thermoelectric materials, which can now be tested experimentally. Thus, the results are very relevant to applications.

- The quality of publications

There are four publications by Tao Fan related to the thesis. In three of them, he is the first author. All publications are in reputable peer-reviewed international journals. The scientific quality of the publications is excellent.

- The summary of issues to be addressed before/during the thesis defense

Below are listed some detailed comments to be addressed directly by modifying the text, unless a discussion is needed.

"In addition, the carrier concentration could change with temperature, whereas we use a fix value in calculation for simplicity." - This sounds like a very crude unphysical approximation. The carrier concentration in semiconductors usually strongly depends on temperature. Clarify why such a crude approximation is considered.

Table 2.1 and other tables - all notations should be clearly explained; even if they seem obvious; κ_{cal_cor} is not obvious at all; is this the value with the scaling factor?

Figure 2.3 - it is confusing; surely the corrected data do not lie on one line; then it is unclear what the red line shows

"Most examples show a bit large difference" -> "... a slightly larger difference"

"the deformation potential theory is a roughly approximation" - "... rough approximation"

"Other process, such as scattering from grain boundary" - "Other processes, ..."

"whereas we use a fix value in calculation for simplicity." - "... a fixed value..."

"Figure 3.1. Maximum power factor as a function of the corresponding carrier concentration for the studied compounds in the temperature range from 300 K to 1000 K..." - it would be good to see particular temperatures for which data are plotted, at least for some (the best) materials; or they can be listed in the caption

Table 3.1 - clarify for which temperature these data are calculated

Conclusions, the part from "Among the novel thermoelectric materials with cubic structure..." till "...therefore their figure of merit can exceed 1 in a wide range of temperatures and carrier concentrations." - I think it would be better to simply list several best predicted thermoelectrics, without relation to crystal structure, for each type (n or p) and temperature range (medium and high), taking into account other important considerations such as non-radioactivity, lower toxicity (I think you have already done this).

Provisional Recommendation

☒ *I recommend that the candidate should defend the thesis by means of a formal thesis defense*

☐ *I recommend that the candidate should defend the thesis by means of a formal thesis defense only after appropriate changes would be introduced in candidate's thesis according to the recommendations of the present report*

☐ *The thesis is not acceptable and I recommend that the candidate be exempt from the formal thesis defense*