

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: Prof. Artem Oganov

Name of the Reviewer: Prof. Alexei Buchachenko

<p><u>X I confirm the absence of any conflict of interest</u></p> <p>(Alternatively, Reviewer can formulate a possible conflict)</p>	<p>Signature:</p> <p>Date: August 8, 2022</p>
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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

Reviewers report should contain the following items:

- Brief evaluation of the thesis quality and overall structure of the dissertation.*
- The relevance of the topic of dissertation work to its actual content*
- The relevance of the methods used in the dissertation*
- The scientific significance of the results obtained and their compliance with the international level and current state of the art*
- The relevance of the obtained results to applications (if applicable)*
- The quality of publications*

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

The thesis submitted by Tao Fan to fulfill the requirements of the Skoltech PhD degree in Materials Science and Engineering develops the theoretical frame for screening and discovery of efficient thermoelectric materials. Practical importance, theoretical and computational challenges of this task, as well as the novelty of the proposed solutions, are well justified and explained in the thesis.

To my opinion, the level of the research presented in the thesis, as well as the way of presentation, is outstanding. First, the goals are clearly set and achieved, not only in terms of the scientific conclusions, but also as the published software. Thus, the thesis presents exhaustive solution of the scientific problem in a self-contained way. Second, the methodology used for calculations of the thermal and electric properties is well justified in the literature review and assessed. Third, rational and original approaches for arranging the workflow for materials discovery are used. Fourth, high potential of the proposed materials discovery frame is convincingly illustrated by application to various classes of relevant compounds, among which the perspective ones are identified. Fifth, the results of the thesis are presented in a logical way and described with scrutiny. The text is well written.

High quality of the work finds a confirmation in the publication list, which consists of four research papers of Q1 level. Among them, publications in *Comp. Phys. Commun.* should be mentioned as certifying the software created as a valuable deliverable.

On this very positive background, I still have some minor comments.

- (1) In sections 2.3.2 and 2.3.3 the author assesses the accuracy of approaches used to compute thermal conductivity and electrical transport properties. Overall assessment is made in terms of RMS averages, which are indeed representative for the task of materials screening. Nevertheless, it could be instructive to discuss absolute uncertainties. Furthermore, there is no information on the reliability of ZT values. They incorporate uncertainties in both thermal and electrical parts in a nonlinear way and one may expect nontrivial variation in their accuracy depending on uncertainties in each counterpart. I think this issues deserves some discussion.
- (2) The text would be benefit from better formatting of the Tables. In particular, Table 3.1 should be formatted as continued on several pages.
- (3) Figures 2.4-2.6 are borrowed from the author's paper in *Comp. Phys. Commun.* It should be indicated in the captions to explain the legend 'this work'.

To conclude, the thesis by Tao Fan is a comprehensive and self-contained work that features high-level science and attests its author as qualified researcher in the field of solid-state physics and computational modeling with excellent programming skills.

Provisional Recommendation

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