

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: Alexander Shapeev

I confirm the absence of any conflict of interest

Date: 13-08-2022

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

Tao Fan's thesis documents the development of methods for evaluating and searching for efficient thermoelectric materials and the results of applying the developed methods. The work on both, the methods and the proposed computationally found promising thermoelectric materials, is at the highest international level.

The structure is adequate: Introduction gives a detailed overview of the subject, including theory and applications for thermoelectric materials and methods of computationally evaluating the efficiency of such materials. Following Introduction is a section about the methodology, borrowed and newly developed by the defendant. Then - a section with the details of the conducted searches for promising thermoelectric materials, and then - a section describing the outcomes of the search. As a result, a number of promising new thermoelectric materials have been computationally identified.

The work was published in four papers in highest-level international journals, out of which in three Tao Fan was the first author. Overall, Tao Fan's thesis is an excellent work, satisfying all the requirements of Skoltech's PhD thesis and I therefore believe that the author's work should be awarded a Skoltech PhD degree upon successful defense.

Some minor remarks include:

1. p.21: The fractions of constituents in $(\text{GeTe})_{0.85}(\text{AgSbTe}_2)_{0.15}$ should be subscripts
2. Equations (2.21) and below: there appear problems with typesetting: subscripts “||” (two parallel lines) seem to be occasionally missing

While reading the thesis I had the following question:

1. What is a typical cost (e.g., in CPU core hours) of evaluating the thermoelectric efficiency of one material.

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