

## 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:

I confirm the absence of any conflict of interest  (Alternatively, Reviewer can formulate a possible conflict)	<b>Date: 17-August-2022</b>
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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

Overall, the topic is good and the thesis draft is in a good shape and nearly qualified for defense.

1, The author gave a good overview of the transport mechanism of electrons and phonons, and also presented the details of calculating the transport properties for screening thermoelectric materials. The codes developed together with this thesis for calculating electric and thermal transports from available crystal structure database by using VASP have been published and are available for public. All of those make the current thesis useful for thermoelectric community.

2, There are a few problems that need to be stressed before the thesis is finalized.

- a) Usually, theoretical Seebeck coefficients ( $S$ ) from calculations show good consistency with experimental values based on earlier observation, including  $S$  itself and its dependence on carrier concentration or temperature. However, Figure 2.8 shows that the calculated  $S$  does not fit experimental values well for many systems. Please double check the issue.
- b) For screening semiconductor thermoelectric materials, band gap is a good indicator for good materials. The current approach uses GGA in PBE to evaluate transport, the reliability of band gap issue should be discussed more carefully, including its correlation to the accuracy of calculated transports. Usually, gap is used as the first indicator to screen good systems. More details should be discussed in the thesis.
- c) Currently, thermal transport, i.e. the lattice thermal conductivity, is mainly based on nonlinear phonon interaction (3 phonons). This is good for many packed systems such as Si or similar systems. But, for Cs- and Ba-containing systems, some loosely packed systems, and/or SnSe-like materials, there may exist rattling modes or phonon interaction beyond 3-phonon scattering. In that way, lattice thermal conductivity should be evaluated in a modified way. Accurate evaluation of this point could be very difficult, but a relatively in-depth discussion for certain materials with this character should be included in the thesis.

#### Provisional Recommendation

**X** 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