Skoltech
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Jury Member Report – Doctor of Philosophy thesis.

Name of Candidate: Artem I. Samtsevich

PhD Program: Materials Science and Engineering

Title of Thesis: Simulation of the mechanisms of solid-solid phase transitions

Supervisor: Prof. Artem Oganov

Date of Thesis Defense: 26 August 2021

Name of the Reviewer: Alexander Shapeev

I confirm the absence of any conflict of interest	**Signature:**  **Date: 22-07-2021**

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 of Artem Samtsevich is an excellent work reporting the development and validation of a novel algorithm of predicting the mechanism of phase transition between two given crystal structures. In my view, the amazing aspect of the algorithm is not that it actually works in sufficiently many cases better than the existing algorithms, but that it involves practical knowledge from very diverse fields as crystallography on the one hand and graph theory on the other hand.

This posed a tough challenge for Artem to concisely describe the algorithm, giving only sufficient pieces of knowledge from different fields of knowledge like graph theory or group theory. I find that Artem did this job well with, however, some space for improvement – see my remarks in the end of the report.

Nevertheless, the thesis quality is very good, the overall structure is adequately chosen to present the algorithm and results of its validation. Methodologically it is very fine work combining methods from different fields. The obtained results are pushing the capabilities of computational materials design to the new level and are definitely at the international level. The work has been published in a number of well-recognized international journals.

In summary, this is an excellent work, satisfying all the requirements of Skoltech's PhD thesis and I therefore believe that the author work should be awarded a Skoltech PhD degree upon the successful defense.

Minor remarks on the manuscript:

1. The quality of English is rather good and I did not trouble understanding almost all the details. However, I advise the author to re-read and fix some of the issues with English, including:
    a. the use of em dash vs en dash vs hyphen,
    b. plurals, tenses, etc.
    c. choice of words (e.g., denoting vs noting)
    d. explaining some of the unusual terminology (like "decomposition of a network by symmetry" (p. 35))
2. Figure 1.1. is slightly misleading: as if MD simulations cannot capture atomic vibrations
3. The algorithmic details, like what is a supernet and subnet, could perhaps be better explained on an example of a crystal (even a toy-2D crystal) by identifying which bonds are part of supernet/subnet.

While reading the thesis I had the following questions left unanswered:

1. I would expect that the transformation between phases, in many cases, would not occur everywhere in the bulk at the same time, but would start somewhere from a nucleus. In other words, one should be concerned about the energy barrier of nucleating a small grain of the phase from the old phase. Can the candidate please comment how relevant would his method be to predict the mechanism and the likelihood of such transformation happening (e.g., by computing the "bulk energy barrier" in eV/atom) in this case.
2. How can experimentalists use the results of this work?

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*