

Jury Member Report – Doctor of Philosophy thesis.

Name of Candidate: Artem Samtsevich

PhD Program: Materials Science and Engineering

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

Supervisor: Professor Artem Oganov

Name of the Reviewer: Professor Xavier GONZE

I confirm the absence of any conflict of interest

Signature:



Date: 26-07-2021

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 PhD thesis by Artem Samtsevich presents a methodology to predict the mechanism for solid-solid phase transitions, and the results of this methodology applied to four different cases of such phase transitions. The methodology has been implemented in a workflow, inside the USPEX code, driving different software applications : first-principles calculations (VASP), variable-cell nudged elastic band optimization (USPEX), topological characterization and search (TOPOS), and A. Samtsevich own developments within USPEX. The capability of this methodology is demonstrated by the successful investigation (and contribution to publications) of the Pnma CrN to a newly predicted hard CrN phase, from $P2_1/c$ -CaCO₃ to $Pm\bar{m}n$ -CaCO₃ (postaragonite) phase, from $I4_1/amd$ -WB to a newly predicted phase WB and andalusite – kyanite – sillimanite transitions in Al₂SiO₅.

The structure of the thesis is clear, with five short preliminary parts (abstract, list of publications, acknowledgments, personal contribution, thesis outline), two useful parts on state-of-the-art and theoretical background (one called introduction and another one on "simulating phase transitions") and then the major part of the thesis, with two chapters : the first to describe the methodology and the second to present applications. Then follows a short part entitled "Conclusion and Future perspectives", and finally the references.

The title of the dissertation and its content match very well. Similarly, the methods used in the thesis are adequate to match the objectives. The results are significant and comply with international standards. It is unfortunate that the methodology part has not been published as such, while three applications have been published, but always as included in larger publications whose first author is not the candidate (until the article 4 is actually published).

The thesis is scientifically sound. Its orientation is clearly methodological, although applications are sufficiently numerous to convince the reader of the adequacy of the methodology. Also, the analysis of the applications is interesting, in terms of bond breaking and formation as well as presentation of the intermediate states.

Based on the above arguments, it is clear that the thesis can be presented at a formal thesis defense.

Still, many adjustments should be done to the manuscript :

(1) I strongly suggest the candidate to separate each chapter from the previous one in the text, and label them explicitly as "Chapter XYZ" in the text. Also, the candidate should number the sections inside the chapters, and possibly should number subsections. The table of content should be updated accordingly.

(2) I find also a bit strange that the "Introduction" chapter also includes two sections that are more advanced than usual introductory material, entitled "Theories of phase transitions" and "Transition State Theory". Perhaps they should be included in Chap. 2, that should then be renamed "Theoretical background" ?

(3) It is not clear whether there is somewhere a list of previous first-principles investigations of solid-solid phase transitions. Actually, methods are listed indeed, but some brief mention of the specific transitions studied in these works might be useful. This is to complete the state of the art : what people were able to do before the current work ? There is actually the mention of one specific system at p25 : graphite to diamond.

(4) Many English mistakes are present (often words are missing), and also the bibliographical references need to be "cleaned" (many need to be completed). Some figures need also to be clarified. To help in this respect, I have noted some of these and will transmit them to the candidate.

Let me reiterate that the overall impression is positive and the above suggestions are aimed at improving the thesis without constituting an obstacle to public presentation.

As such, I recommend the thesis to public PhD defense.



Xavier GONZE, 26 July 2021.

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