

Jury Member Report – Doctor of Philosophy thesis.

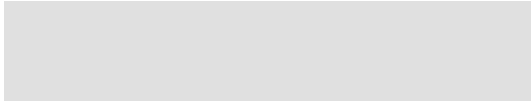
Name of Candidate: Vadim Sotskov

PhD Program: Materials Science and Engineering

Title of Thesis: Data-driven design of multicomponent alloys

Supervisor: Professor Alexander Shapeev

Name of the Reviewer:

| | |
|--|-------------------------|
| I confirm the absence of any conflict of interest  | Date: 09-10-2023 |
|--|-------------------------|

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 thesis is well structured and clearly written. The amount and quality of the work are impressive.

- The relevance of the topic of dissertation work to its actual content

The topic of the thesis is directly related to the content.

- The relevance of the methods used in the dissertation

The candidate developed new methods specifically to solve important scientific problems discussed in the thesis.

- The scientific significance of the results obtained and their compliance with the international level and current state of the art

The candidate has developed a methodology for multicomponent alloys computational design. He wrote the code for on-lattice crystal structure prediction and Monte Carlo sampling. He also applied the developed methodology to several multicomponent alloy systems that are currently discussed in literature. By doing so, the candidate clarified some of the outstanding issues in this field. The work sets a new standard in modelling multicomponent systems, and therefore has a very high scientific significance.

- The relevance of the obtained results to applications (if applicable)

The developed methodology can be used to predict stable multicomponent materials, which is a new frontier in discovery of functional materials with improved properties for various applications.

- The quality of publications

Two papers based on the thesis work were published in respected peer-reviewed international journals indexed in Web of Science database (npj Computational Materials with impact factor >12, and Physical Review Materials). The publications are of very high scientific quality, in collaboration with outstanding Russian and international groups.

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

“In this work I propose a methodology for designing multicomponent alloys using on-lattice modeling. This approach assumes that the simulated system has an ideal lattice with fixed atomic positions.” – Was some relaxation still accounted for by fitting cluster expansion model to relaxed energies?

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