Skoltech
Skolkovo Institute of Science and Technology

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: Artem R. Oganov

I confirm the absence of any conflict of interest (Alternatively, Reviewer can formulate a possible conflict)	**Date: 12-10-2023**

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 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

Vadim Sotskov's PhD thesis presents an excellent, perhaps an exemplary research work. Applying state-of-the-art methods, largely developed by him and his supervisor, Prof. A.V. Shapeev, to interesting and challenging problems of alloy design, Vadim obtained convincing results.

On-lattice machine learning interatomic potentials can give unprecedented level of accuracy. Their combination with Monte Carlo methods allows one to quantitatively explore order-disorder transitions, compute thermodynamic functions (heat capacity, entropy, etc), find ordered ground states, construct phase diagrams. Vadim has developed two novel approaches – (1) for predicting ordered ground states and (2) for predicting order-disorder transitions. He demonstrated reliability and efficiency of these approaches on a number of alloy systems and obtained results that agree nicely with experiment and explain experimental observations at the microscopic level.

Research of this quality would lead to a PhD degree at any top international university. I recommend awarding the PhD degree to Vadim Sotskov without any reservation.

A very minor comment – USPEX method was for the first time developed not in 2013 [Lyakhov et al., 2013], but in 2006 [Oganov & Glass, 2006]. The 2013 paper reports an important further development.

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*