Skoltech
Skolkovo Institute of Science and Technology

# Jury Member Report – Doctor of Philosophy thesis.

**Name of Candidate:** Konstantin Gubaev

**PhD Program:** Materials Science and Engineering

**Title of Thesis:**

Machine-learning interatomic potentials for multicomponent alloys

**Supervisor:** Prof. Alexander Shapeev

**Chair of PhD defense Jury:** Prof. Alexei Buchachenko ***Email***: *a.buchachenko@skoltech.ru*

**Date of Thesis Defense:** 02 October 2019

**Name of the Reviewer:**

| I confirm the absence of any conflict of interest | **Signature:**<br><br>Biswanath Dutta<br><br>**Date: 02-09-2019** |
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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

The topic of the thesis, i.e., Development of machine-learning interatomic potentials for multicomponent alloys is a very active field in state-of-the-art materials science research. The present PhD thesis by Konstantin Gubaev contributes significantly to the ongoing efforts in the development of machine-learning potentials. The thesis contains brief introduction to the topic, overview of state-of-the-art computational methods, thorough description computational methods of the present thesis, achieved results and finally a conclusion and bigger picture associated with the research work. Therefore, the quality and the overall structure of the thesis are very good.

The philosophy of moment tensor potentials and active learning or learning on-the-fly is very promising and can have applications in different areas of materials science and engineering. Therefore, the developed methods and obtained results are really of high quality and state-of-the-art in materials science research. The two published articles related to the thesis are of international standards and highlights the quality of research work performed by Konstantin. Therefore, I strongly believe that Konstantin deserves to get a PhD degree based on the work presented in his thesis.

While reading the thesis, I had difficulties at few instances. I would really appreciate if Konstantin can clarify my doubts on the following issues:

(1) How important is the choice of initial set of configurations for the quality of MTP? Did you try with different set of initial configurations and still ended up with the same "final" training set? Also, how many initial configurations do you typically require? You might provide the numbers for the three studied alloys in sections 4.1.1, 4.1.2 and 4.1.3 respectively.
(2) A related question. How reliable are the MTPs for extrapolation. For instance, will it be possible to see a phase transition (e.g., martensitic transition) if the MTP is trained with data from only one of the phases? This is an example scenario but such a situation of extrapolation can arise in other cases as well.
(3) In the present thesis, the machine learning approach previously developed for single component systems have been extended to multiple component alloys. Can you describe what were the key challenges you faced in this extension and how did you handle those challenges?
(4) In the conclusion, you have mentioned about "long-range interactions" as a limitation. I am curious to know if MTPs can handle short-range ordering? This is important in the context of statements you have mentioned in pages 54-55 for cluster expansion.
(5) What is the technical difficulty of MTPs for magnetic systems? What about systems with interstitial elements such as Carbon or Hydrogen? Can you comment on the applicability of MTP for magnetic systems and systems with interstitial systems?
(6) In page 16, what is the difference between U's in equation (3) and equation (4)? Also, why is the condition j>i in equation (3) necessary?
(7) Last but not least, the thesis should be checked carefully for spelling mistakes and formulations. I have found plenty of mistakes in the thesis.

**Provisional Recommendation**

☒ *I recommend that the candidate should defend the thesis by means of a formal thesis defense*

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| ☐ *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* |