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. Nikolay A. Gippius ***Email:*** *n.gippius@skoltech.ru*

Date of Thesis Defense: 02 October 2019

Name of the Reviewer: Nikolay Gippius

I confirm the absence of any conflict of interest (Alternatively, Reviewer can formulate a possible conflict)	**Signature:**  **Date: 02-09-2019**

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 Konstantin Gubaev describes his research in which he applies machine learning to models of interatomic interaction and test it on two problems, one from chemistry and one from materials science.

The overall structure of the thesis is adequate: it begins by describing the broad picture of the atomistic simulations field, then proceeds to the conventional models of interatomic interaction and leads to the idea of machine-learning potentials being a promising tool for the materials science applications. The applications are provided in the corresponding section, followed by perspectives of the work and concluding remarks.

In his work Konstantin extends the previously developed methodology for single-component potentials to the case of multiple components. Namely, the thesis proposes a special type of machine-learning potentials--the moment tensor potentials (MTPs)--capable of accurate interpolation of the quantum-mechanical calculations data, and an active-learning algorithm for automated training of such potentials. The applications include searching for stable alloys and organic chemistry predictions, and in both these cases MTPs has shown a great effectiveness as an interatomic interaction model. I consider Konstantin's research as an excellent and perspective application of machine-learning techniques to the problems of materials science.

The two thesis-related peer-reviewed papers of Konstantin published in 2018 and 2019 have already accumulated 40 combined citations in Google Scholar, which suggest the relevance of Konstantin's research for the scientific community.

In general the thesis is well-written and understandable, however while reading I have some questions left unanswered:

1. The chemistry application appear to predict properties of equilibrium molecules. Are MTPs able to predict chemical reactions?
2. MTPs compute the interaction energy based on atomic coordinates. What happens if there are atomic charges or spins present in the system?
3. In several places it is mentioned that active learning "effectively detects extrapolation". In what sense do MTPs extrapolate?

Some typos and minor remarks:

p.14 - "Instead, they provide an explicit analytical form with..."

p.20 - "tens of thousands of parameters parameters..."

p.30 - "Figure 5 a" – remove space

p.31 - "During sampling some force field.."

p.31 - "Next, some amount of configurations is picked, corresponding…"

p.32 - "Correctness" is a new unexplained word – maybe "Reliability"?

p.53 "Thus, structural optimization of the training structures.."

p.102 - "Trial-end-error approach..."

p.103 - "Functional form of MIPS..."

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*