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

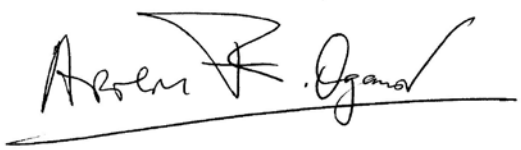
Title of Thesis:

Machine-learning interatomic potentials for multicomponent alloys

Supervisor: Prof. Alexander Shapeev

Date of Thesis Defense: 02 October 2019

Name of the Reviewer:

I confirm the absence of any conflict of interest (Alternatively, Reviewer can formulate a possible conflict)	**Signature:**  **Date: 10-09-2019**

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

This is a pioneering work with far-reaching implications for materials science, physics and chemistry. Machine learning revolution has deeply impacted these disciplines, largely through enabling an accurate and computationally convenient representation of interatomic interactions in condensed matter. This approach (in particular, through the use of G. Csanyi's GAP approach and A. Shapeev's MLIP method) has already shown its practical value for elemental crystals and binary compounds, but as the number of atomic types increases, the number of parameters and the size of the training dataset should seemingly increase exponentially, rendering this approach practically useless for complex systems.

K. Gubaev has shown how to overcome this bottleneck and reach scaling lower than quadratic without introducing any additional approximations. This gives a practical recipe for accurate calculations. Present thesis gives examples of solving highly non-trivial problems with this approach. For example, new structures were predicted: Cu_5Pd, Co_3Nb_2V, $AlNi_2$, $AlNi_{11}$, $AlNi_9Ti_2$. Good accuracy in representing atomization energies was shown for organic molecules containing C, H, O, N, F. These results are extremely impressive. But going beyond representation of the energy (which is a short-ranged property, determined mostly by local interactions), K. Gubaev showed that his approach can be used for predicting non-local properties, such as HOMO-LUMO gaps.

As I wrote above, I consider K. Gubaev's PhD thesis as an extremely valuable scientific work of high scholarly level. There is no doubt that K. Gubaev deserves the PhD degree of Skoltech or any top university.

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*