Skoltech
Skolkovo Institute of Science and Technology

Jury Member Report – Doctor of Philosophy thesis.

Name of Candidate: ZAHED ALLAHYARI

PhD Program: Materials Science and Engineering

Title of Thesis: COEVOLUTIONARY SEARCH FOR MATERIALS WITH OPTIMAL PROPERTIES IN THE SPACE OF BINARY SYSTEMS

Supervisor: Prof. Artem Oganov

Co-advisor:

Chair of PhD defense Jury: Prof. Keith Stevenson   *Email*: k.stevenson@skoltech.ru

Date of Thesis Defense:

Name of the Reviewer: Prof. Prof. Keith Stevenson

X I confirm the absence of any conflict of interest	Signature:
(Alternatively, Reviewer can formulate a possible conflict)	*Keith J Stev*
	Date: June 6, 2020

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*

I am writing this letter to provide an evaluation of Zahed Allahyari on his original creative work (i.e. thesis) entitled "COEVOLUTIONARY SEARCH FOR MATERIALS WITH OPTIMAL PROPERTIES IN THE SPACE OF BINARY SYSTEMS," in the completion of PhD requirements at Skoltech.

Overall, his thesis contains novel and important work in the rapidly developed field of the computational structure and materials prediction. The thesis is arranged into main components: Introduction (Chaps. 1,2), main part describing the approaches developed and applied to efficient structure and materials screening (Chaps. 3-5), example of the search for hard and superhard materials (Chap. 6) and concluding Chap.7. Appendices clarify the implementation of the computational schemes and attest the workload.

The introductory part provides the basics of computational structure and materials predictions and describes how the related approaches are implemented in the USPEX code developed and supported by the group. It does not contain detailed literature review and analysis emphasizing the common problems and one of the possible directions to their solutions. It is, however, tolerable as the novel search algorithms are essentially based on the approaches and utilities implemented in USPEX. The theoretical part describes the essence and implementation of two advanced approaches. One, based on the Pareto optimality, permits one multi-objective searches for structures and materials with more than one desirable properties. Such tasks are inherent to Materials Science and development of realistic computational methods are highly demanded and emerging. Another, called as Mendelevian Search, provides the hints to more efficient structure and materials screening by preselecting the most prospective chemical components. Such a selection is at the core of Chemistry and Material Science and is routinely used in many labs on the daily basis following the fundamental chemical principles and intuition. For those who do such work the concepts of Mendeleev number or Mendeleev space sounds a bit excessive. On the other hand, the thesis evidences that the proposed approach brings significant benefits in terms of the search efficiency. Applications to hard and superhard materials search considered in Chap. 6 confirm the reliability of the methods by comparison with available experimental data. Conclusions correctly feature main research findings presented in the thesis.

The scientific outcomes are reflected in 4 scientific papers and one book chapter. Most of the papers are published or accepted in high impact factor journals. Author contributions to the work are clearly outlined in the beginning of the thesis.

Overall this thesis work provides substantial development of the computational methods of structure and materials prediction towards realistic practical applications. Zahed has done impressive original work and addresses important challenges of this field.

Considering his performance in original research achievements, I recommend the acceptance of his PhD thesis as is, perhaps with further proofreading for typos and formatting inaccuracies.

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*