Skoltech
Skolkovo Institute of Science and Technology

# Jury Member Report – Doctor of Philosophy thesis.

**Name of Candidate: DMITRII V. SEMENOK**

**PhD Program:** Materials Science and Engineering

**Title of Thesis: COMPUTATIONAL DESIGN OF NEW SUPERCONDUCTING MATERIALS AND THEIR TARGETED EXPERIMENTAL SYNTHESIS**

**Supervisor:** Profs. Artem R. Oganov, Alexander G. Kvashnin

**Name of the Reviewer:** Prof. Alexei Buchachenko

| | |
|---|---|
| **X I confirm the absence of any conflict of interest**<br><br>(Alternatively, Reviewer can formulate a possible conflict) | **Signature:**<br><br>**Date: August 13, 2022** |

*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 submitted by Dmitrii Semenok to fulfill the requirements of the Skoltech PhD degree in Materials Science and Engineering lies in the field of high-pressure metal polyhydrides, their synthesis, characterization of structure and electronic properties, as well as the theoretical and computational approaches for predictions of perspective phases and compositions and understanding of their properties behind emergence of the superconductivity. This field is less than 10 years old, but, despite numerous technical complications with high-pressure synthesis and structure characterization, develops vividly, leading to many new discoveries and successes in pushing the critical superconductivity temperature up and the pressure down.

My main impression is that this work goes beyond what we usually expect from the PhD thesis.

First, the scholarity impact of the thesis is very high, consisting of 5 research papers published in Q1 journals in 2020-21, with almost 300 (!) cumulative citations. Three influential papers appeared in 2021 during the thesis preparation, including one in Nature Communications and one in Physical Review Letters. The reference list includes 8 more papers co-authored by Dmitrii, indicating his prior contribution to the field. As a result, field-weighted citation impact made by Dmitrii to the quite broad topic ``Crystal Structure; Superconductivity; BCS Theory`` approaches 6.7, while his h-index – 13 (Scopus). It is by far not typical to a PhD program graduate. Furthermore, Dmitrii combines advanced research skills in both experiment and theory, both not routine for his research field, including the whole cycle of high-pressure synthesis, structure characterization using different synchrotron facilities, modern approaches to crystal structure predictions using the evolutionary algorithm conjugated with density functional theory calculations and models and theories of electronic properties that determine superconductivity and magnetic field effects.

Second, the thesis not only reports remarkable progress reached for each system/class of systems studied, but also provides significant contribution in the physical understanding of the mechanisms behind superconductivity or its suppression. Very simple but instructive analogy of polyhydride properties with the properties of bulk metals is one example. Chapter 6, that present an overview of the superconducting properties of polyhydrides across the Periodic table provides more examples and determines the state of the art in the field.

Third, the thesis is very well and logically written. I would specifically acknowledge the introductory sections for each chapter that emphasize current state of the art, challenging problems and particular research goals, thus better placing each piece in the context of the thesis and making its content more transparent. Overall, the style used makes the reading smooth and interesting even for a non-specialist. Appendix summarizes theoretical details and supplementary data in a useful way.

With this high assessment, I have little to recommend for improvement. Perhaps adding a list of ``other author`s publications relevant to the thesis topic`` after page 4 is instructive to emphasize overall impact of the author in the field. I would also add DOI in the for-thesis

publication list, to comply with publisher`s permission for reusing materials in the dissertations. Reference 46 looks funny – better to put it ``unpublished``. Formatting inaccuracies, mostly in the tables, are worthy of fixing.

Just for curiosity, in section 3.3, the anomalously low Tc for YH6, which cannot be explained by standard models, is emphasized. It would be interesting to discuss at the defense if any new ideas, hints or data have been emerged after thesis completion.

I strongly recommend the thesis for the public PhD defense at Skolkovo Institute of Science and Technology.

**Provisional Recommendation**

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