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Jury Member Report – Doctor of Philosophy thesis.

Name of Candidate: Dmitrii Semenok

PhD Program: Materials Science and Engineering

Title of Thesis: Computational design of new superconducting materials and their targeted experimental synthesis

Supervisor: Professor Artem Oganov

Co-supervisor: Assistant Professor Alexander Kvashnin

Name of the Reviewer: Prof. Haiyang Niu, Northwestern Polytechnical University (haiyang.niu@nwpu.edu.cn)

I confirm the absence of any conflict of interest (Alternatively, Reviewer can formulate a possible conflict)	**Date: 13-August-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

Brief evaluation of the thesis quality and overall structure of the dissertation

The dissertation of Dmitrii Semenok is well-written, with a lot of novel and important scientific findings. The thesis consists of an introduction (Chapter 1), five chapters, a conclusion, a list of references, and an appendix. The research background, the current dissertation's goal and the approaches used by the author are clearly presented in the Introduction Chapter.

In Chapter 2, the synthesis and superconductivity of the thorium polyhydrides are presented by the author. The thorium hydrides ThH_{10} and ThH_9 were predicted theoretically in 2018, before their experimental discovery, which is a proof of the predictive power of the density functional theory, crystal structure prediction algorithm and the Bardeen–Cooper–Schrieffer theory of superconductivity.

In Chapter 3, the author presents a study of the high temperature superconductivity in the yttrium–hydrogen system. Importantly the experimental synthesis of YH_4, YH_6, and YH_9 and their superconducting properties are discussed. The synthesized YH_6 and YH_9 polyhydrides exhibit high-temperature superconductivity at 224 to 243 K.

In Chapter 4, The superconductivity, magnetic properties of europium superhydrides are discussed. It shown that europium hydrides do not exhibit superconducting properties due to the anisotropic scattering centers. The magnetic properties and the underlying physical origin are discussed in detail.

In Chapter 5, the author has investigated the ternary lanthanum–yttrium–hydrogen system. The importance of explore ternary system is discussed. in which La and Y form a solid solution metal sublattice; this study is the first of the kind for superhydrides. In detail, the superconducting properties of the ternary lanthanum–yttrium–hydrogen system and a few ternary compounds are investigated.

In Chapter 6, the underlying principle of the superconducting properties in binary and ternary metal polyhydrides are discussed. The rules might be used to predict the maximum critical temperature in binary and ternary systems based on only the knowledge of the hydride-forming elements, which is important to the future of this field.

To summarise, Dmitrii Semenok's dissertation presents a comprehensive investigation of many novel superconducting compounds, and the physical interpretation of the results. The research has adopted advanced experimental and theoretical approaches.

Relevance of the topic of the dissertation work to its actual content

The dissertation presented by Dmitrii Semenok "Computational design of new superconducting materials and their targeted experimental synthesis" focuses on theoretical and experimental studies of the superconducting properties of polyhydrides at high pressures. All the chapters, including all the actual content in the dissertation is strongly relevant to the topic of the dissertation.

Relevance of the methods used in the dissertation

The methods, both the experimental and theoretical, used in the dissertation is well described and closed relevance to all the results presented. The details of the methods make the dissertation reproducible.

Scientific significance of the obtained results and their compliance with the international level and current state of the art

The results, I would prefer to say, the discoveries, presented in the dissertation is in world-class level, which is both scientifically novel and methodological important. To be more specific, the discoveries of the superconducting thorium–hydrogen compounds, yttrium-hydrogen compounds are novel to this field, and the Tc of ThH10, YH6 and YH9 can reach to 161, 224-227, and 237-243 K at high pressure, respectively. In addition, the ternary system La-Y-H system is well investigated, with a record Tc 253 K, which shadow lights to the future development of this field. Furthermore, the author discussed the general rule underlying the superconducting properties of binary and ternary metal polyhydrides, which is predictable to the discovery of more advanced superconductors. To summarize, I would like to say the findings are ranking in the top-list of all the discoveries in the field, which is both state of art and inspiring.

Relevance of the obtained results to applications

The results in this dissertation is expected to guide for the discovery of new high-temperature superconducting hydrides at high pressures, especially in ternary systems.

Quality of publications

The main results of the dissertation have been published in five scientific papers in high-quality peer-reviewed journals. For any of these publications, it is extremely competitive and has a very high impact around the world.

In total, the dissertation of Dmitrii Semenok, "Computational design of new superconducting materials and their targeted experimental synthesis", is a complete research which meets the requirements for awarding a PhD degree according to the criteria of relevance, scientific novelty, and validity and reliability of the conclusions. I would say, Dmitrii Semenok should be awarded a PhD degree.

Summary of the issues to be addressed before the thesis defense

The following remarks can be made on the content of the thesis:

1. The author is suggested to add how exactly Tc is calculated based on the BCS-Migdal-Eliashberg theory in Chapter 1.
2. A few subtitles are suggested to be added to make the thesis more readable, especially in Chapter 1.
3. All the computational and experimental setups to reproduce the findings should be given.

4. The correspondence between column 2 and 3 is not clear in Table 4.
5. The "75 atom%" on page 60 should be "75 at%".
6. Please check the font type of letter "K" on pages 81-82.
7. For those structures discovered both in theoretical predictions and experiments, the comparisons of structural details between experiments and calculations are suggested to be added.

These remarks do not reduce the significance of the obtained results and do not affect the overall positive evaluation of Dmitrii Semenok's dissertation.

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*