Skoltech
Skolkovo Institute of Science and Technology

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: Professor Evgeny Antipov

I confirm the absence of any conflict of interest (Alternatively, Reviewer can formulate a possible conflict)	**Date: 09-08-2022**

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 Ph.D. thesis of Dmitrii Semenok consists of an introduction, five chapters, a conclusion, a list of references, and an appendix. The goal, main objectives, and the novelty of obtained results are well described and explained in the introduction. In Chapter 2, the author describes the synthesis of thorium polyhydrides and their transport properties, while Chapter 3 presents a study of the yttrium–hydrogen system at pressures up to 213 GPa, including the experimental synthesis of YH_4, YH_6, and YH_9, and the investigation of their superconducting properties. In Chapter 4, Dmitrii Semenok discusses hydrides of lanthanides, and pays a special attention to Eu-based materials which does not exhibit superconducting properties, and provides a plausible explanation of this phenomenon. In Chapter 5 the author describes an investigation of the ternary lanthanum–yttrium–hydrogen system. In Chapter 6, the author considers the problem of an appearance of the superconducting properties in binary and ternary polyhydrides. He suggested the rules making possible to predict superconductivity in such materials.

The dissertation of Dmitrii Semenok is focused on superconductivity in polyhydrides at extremely high pressures. The main goal is to predict a superconductivity in polyhydrides by theoretical methods (DFT calculations, an evolutionary search for phases under high pressure, and calculations of the band structure and electron–phonon interaction) followed by experimental verification including their synthesis under high pressure and reliable methods of investigation.

The obtained results are reliable and have a significant novelty:

1. The author found new thorium hydrides under high pressures and one of this compound exhibits a superconductivity at T_C = 161 K under 170 GPa.
2. The formation of europium, praseodymium, and neodymium hydrides were studied in detail. It was shown that these hydrides do not exhibit superconductivity and the explanation of this phenomenon was proposed.
3. It was established the formation of a solid solution in metal sublattices with a random distribution of La–Y and La–Nd atoms in ternary hydrides of these elements, and the superconducting transition at 253 K was found in the La,Y hydride.
4. The author thoroughly investigated the appearance of superconductivity in ternary and binary metal hydrides. It was concluded that particular metal hydrides (with one or two d electrons or containing alkaline-earth metals) are the most promising for superconductivity.

The results of the research can be used as a basis for obtaining new high-temperature superconducting hydrides at high pressures.

The main results of the thesis have been published in five papers in high-quality journals, and the author has received a patent. The results of the thesis have been presented at several international conferences and seminars.

The dissertation of Dmitrii Semenok is a complete original research meeting the necessary requirements for awarding a PhD degree.

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

1. Why different chemical formulas (Th4H15 and Th16H60) are used for the same compound as well as Th4O8 instead of ThO2?

2. How the author can explain the coexistence of ThO2 and Th4H15 in the samples after synthesis?

3. What does it mean: "The superconducting properties of cerium hydrides are weaker than those of thorium hydrides (p. 57)?

4. What are the La/Y ratios in the (La,Y)H10 and (La,Y)H6 compounds (p.109)? Did the author try to prepare these compounds with another La/Y ratios?

These remarks do not reduce the significance of the obtained results and do not affect the overall very positive evaluation of Dmitrii Semenok's dissertation. This thesis represents a significant step in understanding of superconductivity in hydrides. Dmitrii Semenok has done an outstanding original work and addresses many challenges of this field. The PhD student Dmitrii Semenok deserves to be awarded a PhD degree.

Provisional Recommendation

X *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*