Skoltech
Skolkovo Institute of Science and Technology

Jury Member Report – Doctor of Philosophy thesis.

Name of Candidate: Evgeny Iakovlev

PhD Program: Mathematics and Mechanics

Title of Thesis: Multiscale modeling of graphene nanobubbles

Supervisor: Professor Iskander Akhatov

Co-supervisor: Petr Zhilyaev

Name of the Reviewer: Aslan Kasimov, Assoc. Prof.

I confirm the absence of any conflict of interest	**Date: Sep. 10, 2021**

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:

The dissertation contains results that reflect high quality scientific research in the area of modeling heterogeneous nanostructures involving graphene. The dissertation is written around the published papers, the latter included in their final published form. While this style is not common, it may be acceptable as long as there is a common theme among various papers and the organization is logically coherent. In my opinion, it is the case here.

The content of the dissertation is completely in agreement with the chosen topic.

The methods used are the state-of-the-art simulation tools of molecular dynamics. In addition, methods of continuum mechanics and density functional theory are also used to get further

insight into the nature of the graphene nanobubbles and of various gases trapped in the bubbles beyond that provided by the MD simulations.

Scientific results are of substantial significance which is also reflected in the quality of the journals in which they are published. There are new physical effects discovered such as the solid state of argon when it is trapped inside a carbon nanobubble at thermodynamic conditions corresponding to liquid state under normal conditions. This new phenomenon is attributed to the strong confinement provided by the bubble. Furthermore, in this work there is a theoretical prediction made about the existence of unstable (or "forbidden") radii of the graphene nanobubbles.

The relevance of these results to applications is only briefly touched on, but clearly they are relevant in various areas of technology dealing with graphene nanostructures in which a trapped matter occurs.

Publications are of good quality and appear in serious recognized journals in the area and in good conference proceedings.

Undoubtedly, the science behind the dissertation work is clear and of interest to the subject area. However, the text might benefit from some improvements, especially concerning various language issues. To mention a few:

p. 16: "large pokets"

p. 17: "useful to use", "this values"

p. 27: "nobel gases"

p. 32: "phenomenon of universal shape scaling is approved", "elastic modules"

pp. 81-82: Why the red text?

p. 85: "the formation of graphene nanobubbles are disclosed"

p. 86: The Glossary is missing a lot of other abbreviations actually used in the text: cDFT, GNB, FMT, LAMMPS, CNT, etc.

Overall, the work should be evaluated as an excellent achievement deserving the PhD degree.

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*