Skoltech
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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: Denis Bandurin

I confirm the absence of any conflict of interest (Alternatively, Reviewer can formulate a possible conflict)	**Date: 05-08-2021**

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:

- 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 PhD thesis of Evgeny Iakovlev “Multiscale modeling of graphene nanobubbles” covers molecular dynamics simulation of graphene nanobubbles with radii less than 30 nm and continuum approach, which allows to model bubble with any radius. The motivation of this study came from experimental work, where special properties of graphene nanobubbles were discovered. In the thesis morphology of the bubbles is investigated as well as the properties and phase state of trapped material. The author performed a qualitative comparison with experimental studies.

The thesis consists of 4 parts. The first one is the introduction, where the motivation and goals are presented. Then the comprehensive literature review is following with the history of graphene nanobubbles studies, also molecular dynamics methods and used interatomic potential are described. The thesis objectives consist of 6 chapters. Each one is represented by the article in peer review journal. Before each chapter, there is a small introduction that connects the parts. The conclusion finalizes the thesis, where a summary and outlook are presented. In general, the thesis is well written and well structured, and chapters are presented in logical order.

In the work, the molecular dynamics method is used for the first part of the research, which is an acknowledged method in modern science for studying materials with nano-size scale. In the second part, the semi-analytical approach is used, that based on the theory of elasticity of membranes. Also, the author used well-studied NIST equations of state of matter to describe the behavior of the trapped substance. Finally, the Chebyshev polynomials are used to represent the shape of the bubble and displacements in the graphene sheet – the convenient method to represent the functionals. Each method is described enough to understand and reproduce the calculations.

The provided models are able to predict the shape of the bubble as well as the state of the trapped matter. Also, the behavior of the substance inside the bubble is studied. Although the theoretical models were developed previously in [Khestanova, et al. Nat. commun. 7.1 (2016): 1-10.], they did not consider the state of trapped matter. Also, previously undiscovered phenomena are described, such as crystallization of argon inside the bubble at the conditions where bulk argon is liquid, and ‘forbidden regions’ – the ranges of radii of graphene nanobubbles which separates the bubbles with liquid matter and bubbles with gas state of matter. All that results prove that the work is done at a sufficient level for the defense.

The obtained results have been published in 6 articles. There are 4 articles in Q1 journals (Scientific Reports, Nanotechnology, Physical Chemistry Chemical Physics, The Journal of Chemical Physics) and 2 in Q3 journal (Journal of Physics: Conf. Series). All papers are of high quality. I recommend the author of the thesis for the Ph. D. degree, the candidate should defend the thesis by means of a formal thesis defense.

I would recommend:

- to add the contribution section before each chapter.

- to fix imprecise wording in the text. For example on p.11: “This research shows that matter behavior in confinement significantly differs from bulk matter.” It should be, to keep the logic: “This research shows that matter behavior in confinement significantly differs from bulk matter behavior.” Or, on p. 19: “Another work studied pseudo-magnetic field in graphene nanobubbles using MD method.” The work cannot study. There are more in the text. It should be fixed.

- to delete/change 1.8 section. What is the purpose of this section? It is very confusing. It is a mix of research questions and highlights of the results.

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*