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: Prof. Dr. Nikolaus A. Adams, Technische Universität München

I confirm the absence of any conflict of interest (Alternatively, Reviewer can formulate a possible conflict)	**Date: 26.08.2021**

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

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

  The thesis has the form of a cumulative (publication based thesis) with the according structure. Summary and publications are well readable. Formal quality is good, technical quality is excellent.
  The journal publications are of very-high to excellent quality with respect to the field.

- The relevance of the topic of dissertation work to its actual content

  A continuum model that supplements MD investigations is crucial to bridge fundamental research on graphene nanobubbles towards applications. Of particular practical relevance Is the interaction between substrate, graphene and enclosed matter. The model is based on extensive MD invetigations and thus extends these very fundamental studies towards practical configurations. The work of the thesis can be considered as a breakthrough contribution in practical understanding of graphene nanobubbles.

- The relevance of the methods used in the dissertation

  The investigations of physical configurations are based on energy-equilibrium criteria, where properties are derived from first principles (molecular dynamics simulations) and encoded into a numerical algorithm that delivers the equilibrium state. For MD the state of the art implementation LAMPPS is used. An extension is developed where the enclosed fluid state is modeled from a density functional, taking into account the various interactions, which delivers a total-energy estimate for the enclosed fluid.

- The scientific significance of the results obtained and their compliance with the international level and current state of the art

  The results are innovative and constitute a breakthrough in the understanding of graphene nanobubbles with contained fluid. In particular they have clarified the state of the enclosed matter and revealed details on phase transitions.

- The relevance of the obtained results to applications (if applicable)

  As nanobubbles are of high technical interest, the thesis constitutes an important step towards technological applications.

- The quality of publications

  The quality of publications is excellent. The results have been published in the leading journals of the research field.

No issues to be addressed further.

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*