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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: Ekaterina Khestanova

I confirm the absence of any conflict of interest	**Date: 17-08-2021**

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 thesis "Multiscale modeling of graphene nanobubbles" summarizes the results of numerical and analytical investigation of the properties of graphene nanobubbles. The text is well composed and comprehensively written. The structure of the thesis consists of a number of peer-reviewed publications by the candidate with the introductory passages which link the chapters into a connected manuscript. The format makes the thesis concise and focused on the main results which is valuable.

As fairly pointed out by the author of the thesis, nanobubbles formed by the matter confined between the layers of van der Waals heterostructures has received considerable attention recently. This is due to the simplicity of obtaining such nanobubbles and, at the same time, their versatility in terms of possible effects both on the confined matter and the atomically thin membrane outlining the trapped substance. This versatility is evidenced by the large variety of experimental approaches taken to study this system, ranging from scanning atomic force microscopy, tunnelling spectroscopy to optical methods. However, the truly nanoscopic sizes of the van der Waals nanobubbles limit the experimental studies only to the high spatial resolution techniques. On the other hand, this makes such nanobubbles a perfect system to study by means of molecular dynamics simulations and to link them with continuous models describing atomically thin membranes confining thermodynamically large quantities of trapped matter. The latter approach has been taken by the author of the thesis and has been successful as evidenced by the considerable number of important scientific results and publications.

The author of the thesis has used molecular dynamics simulations as the major tool for his numerical studies. In the recent years this method has become one of the workhorses in material science, however, it requires the properly chosen interatomic potentials to begin with. The author of the thesis considers a few main potentials such as Tersof, AIREBO, TraPPE-UA and explains the main application fields of each. Furthermore, Yakovlev applies a continuum approach, where the Young´s modulus of the membrane is already input into the model and nanobubbles of any radius can be described in this way. This approach simplifies calculations and allows to estimate adhesion energies between the constituents of the nanobubble and its contents. It also allowed the author to predict new phenomena such as a "forbidden zone" of sizes in the argon-filled graphene nanobubbles, which is interesting on its own but still awaits experimental confirmation. Although Ar-filled nanobubbles have been obtained experimentally, the more frequent type of molecules trapped inside graphene nanobubbles are hydrocarbons. Remarkably, the thesis also considers this type of molecules and shows the results of ethane-filled nanobubbles modelling, linking it to the possible applications for hydrocarbons storage and processing.

The overall quality of publications is high as evidenced by their citations. Importantly, the publications contain experimentally verifiable predictions which makes the developed theoretical and numerical analysis exceptionally valuable to the field.

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*