Přírodovědecká fakulta
Faculty of Science

Jihočeská univerzita v Českých Budějovicích
University of South Bohemia in České Budějovice

OPPONENT'S REVIEW ON BACHELOR THESIS

Name of the student: Stefan Ferlin

Thesis title: The Interaction of Graphene Oxide with Humic Acids, a Computational Study

Supervisor: Dr. Babak Minofar, Ph.D.

Referee: Assoc. Prof. Martin Kabeláč
Referee`s affiliation: **Institute of Chemistry, Faculty of Science, University of South Bohemia**

	Point scale[1]	Points
(1) FORMAL REQUIREMENTS		
Extent of the thesis (for bachelor theses min. 18 pages, for masters theses min. 25 pages), **balanced length of the thesis parts** (recommended length of the theoretical part is max. 1/3 of the total length), **logical structure of the thesis**	0-3	3
Quality of the theoretical part (review) (number and relevancy of the references, recency of the references)	0-3	2
Accuracy in citing of the references (presence of uncited sources, uniform style of the references, use of correct journal titles and abbreviations)	0-3	1
Graphic layout of the text and of the figures/tables	0-3	2
Quality of the annotation	0-3	1
Language and stylistics, complying with the valid terminology	0-3	2
Accuracy and completeness of figures/tables legends (clarity without reading the rest of the text, explanation of the symbols and labeling, indication of the units)	0-3	1
Formal requirements – points in total		12
(2) PRACTICAL REQUIREMENTS		
Clarity and fulfillment of the aims	0-3	2
Ability to understand the results, their interpretation, and clarity of the results, discussion, and conclusions	0-3	1
Discussion quality – interpretation of the results and their discussion with the literature (absence of discussion with the literature is not acceptable)	0-3	1
Logic in the course of the experimental work	0-3	3
Completeness of the description of the used techniques	0-3	0

[1] Mark as: 0-unsatisfactory, 1-satisfactory, 2-average, 3-excellent.

Experimental difficulty of the thesis, independence in experimental work	0-3	2
Quality of experimental data presentation	0-3	2
The use of up-to-date techniques	0-3	3
Contribution of the thesis to the knowledge in the field and possibility to publish the results (after eventual supplementary experiments)	0-3	2
Practical requirements – points in total		16
POINTS IN TOTAL (MAX/AWARDED)	**48**	**(28)[2]**

Comments of the reviewer on the student and the thesis:

The bachelor thesis of Stefan Ferlin entitled "The Interaction of Graphene Oxide with Humic Acids, a Computational Study" is dedicated to a hot topic of water remediation from organic pollutants. The author used a molecular dynamics procedure for study of such problematic.

The Introductory part is dedicated to studied systems, description of the noncovalent interactions and the theoretical background of used technique and a brief description of current state of research follows. This section is written clearly and comprehensibly.

I found a Methods section as a major flaw of this thesis. This part is written rather like a general tutorial how to run the simulations, what would be, of course, beneficial for followers in this work, on the other hand, any information about the simulation setup conditions, force field used, 2D pictures of studied compounds, pH and ionization states of humic acids etc. are completely missing in those paragraphs. This means that the work cannot be reproduced by other scientists. As well as I did not find some details, how the analysis of the results was provided.

The comparison of abilities of different humic acids to bind to graphene oxide based on measurement of distances of certain atoms from the surface is described in the Results section.

The Discussion and Conclusion seems to me written in hurry and it is too short (together one page of text only) and too shallow and it would deserve to be extended at least for comparison of studied compounds on graphene.

Suggestions and questions, to which the student has to answer during the defense. Mistakes, which the students should avoid in the future:

Suggestions and comments

- p.5 Description of Figure 1. Better "typical" than "average" formula of HA
- Mathematical equations should be numbered for lucidity.
- Formats of citations should be unified (they are numbered in the first half of work, whereas in the second part the names and year of publication are used).
- p.18, section 4.1. All programs used in the work should be cited as well.
- p.20. last line: *-np* option does not mean the position of ions , but the number of positive ions
- some misspells in the text (mistery – should be mystery, confirmations- should be conformations, etc.)

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[2] Enter the number of points awarded.

Questions:

- Fig. 4 (p. 10) shows the occurrence of lots of epoxide bridges and the presence of hydroxyl groups in the central part (not only in the edges like in the model) in a common structure of graphene oxide. Why these functional groups were not used in a model studied by the author? It seems to me that the middle part of the graphene oxide layer rather resembles the pure graphene...

- p. 12. *Overlap of electron-dense molecules can cause short range penetration... and damping effects"* Please explain , what do you mean by this terms in given sentence.

- p.18. "*PACKMOL software used to create a point of origin in MD and makes it possible to create confined spaces.*" I did not catch a meaning of this program for MD simulations. Please explain.

- How the distance between the aromatic ring and graphene oxide layer was defined? The definition is very loose in the text. The measurement between polar groups of HA and graphene oxide

- p.30. Please explain possible sources of discrepancies between your findings and Ref. 20.

Conclusion:

In conclusion, I r e c o m m e n d the thesis for the defense and I suggest the grade 3 .[3]

In **Budweis** Jan 17th 2020 Assoc. Prof. Martin Kabeláč

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signature

[3] You can suggest a grade, which can be modified during the defense based on the presentation. However, if the reviewer is not present at the defense, the grade will not be counted. Grades: excellent (1). Very good (2), Good (3), Unsatisfactory/failed (4).