

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

## SUPERVISOR'S STATEMENT ON BACHELOR THESIS

Name of the student: Stefan Ferlin

Study program:

**Biological Chemistry** 

Department/Institute:

**Institute of Chemistry** 

Thesis title:

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

Supervisor:

MSc. Babak Minofar, Ph.D.

Supervisor's affiliation:

University of South Bohemia, Institute of Chemistry

	Point scale <sup>1</sup>	Points
(1) FORMAL REQUIREMENTS		
Formal and graphical quality of the thesis	0-3	2
Ability to work with literature	0-3	3
Language and stylistics	0-3	2
Formal requirements – points in total		7
(2) PRACTICAL REQUIREMENTS		
Fulfillment of the aims	0-3	3
Ability to understand the results, their interpretation, and clarity of the results, discussion and conclusions	, 0-3	2
Discussion quality – interpretation of results and their discussion with the literature	0-3	2
Experimental difficulty of the thesis, independence in experimental work	0-3	3
Contribution of the thesis to the knowledge in the field and the possibility to publish the results (after eventual supplementary experiments)	0-3	3
Practical requirements – points in total		13

POINTS IN TOTAL (MAX/AWARDED)	24	20
POINTS IN TOTAL (MAX/AWARDED)	24	20

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

## Comments of the supervisor on the student and the thesis:

Stefan started his work on the interaction of Graphene Oxide (GO) with humic acids in autumn 2017. The purpose of the project was to study the interaction of humic acids with carbon based materials particularly with graphene oxide. As graphene oxide become well used in many applications therefore the can get to natural waters and wastewaters thus understanding the interaction with humic acids is crucial. In his work, Stefan studied the interaction of GO with different models of humic acids by classical molecular (MD) simulations.

Stefan enthusiastically started to work on the project and learnt very fast how to work with Linux operating system, also the started to study the basic information about computational methods such as molecular dynamics very fast. He started to work independently on the project and he could do the calculations both in Austria via Linux platforms. By his work, Stefan has found that there are different interactions on the adoption of humic acids at the surface of GO where the interactions belong to weak interactions such as stacking and hydrogen bonding interactions. His findings can bring new insights and applications of GO in environmental applications such as water and wastewater technology and removal pollutants from water.

## Conclusion:

In conclusion, I highly

recommend

the thesis for the defense.

In České Budějovice date 1.2.2020

signature