



SUPERVISOR'S STATEMENT ON BACHELOR THESIS

Name of the student: Ivan Khodonovych
Study program: Biological Chemistry
Department/Institute: Institute of Chemistry
Thesis title: Computational study of greenhouse gas adsorption on biochar

Supervisor: MSc. Babak Minofar, Ph.D.
Supervisor's affiliation: University of South Bohemia, Institute of Chemistry

	Point scale ¹	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	3
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	2
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

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

Comments of the supervisor on the student and the thesis:

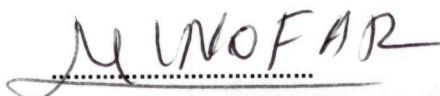
Ivan has started his work on this project in autumn 2017. The main aim of the project is to study the interaction of greenhouse gas such as CH₄, CO₂ and N₂O with different models of biochar by classical molecular dynamics (MD) simulations.

Ivan enthusiastically started to work on the project after discussion with whether he would like to work on computational chemistry related project. He learnt fast how to work with new 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 calculation not only in university in Czech but also performing the calculations via Linux platforms in Austria. By his work, Ivan has found the origin and nature of the interactions which are involved in the adsorption of greenhouse gas at the surface of biochar which can help to design cheap materials such as biochar for environmental applications.

Conclusion:

In conclusion, I highly
r e c o m m e n d
the thesis for the defense.

In **České Budějovice** date **1.2.2020**



signature