Přírodovědecká fakulta
Faculty of Science

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

Supervisor's report on the doctoral thesis
"Application of Electronic Continuum Correction to Molecular Simulations of Nano/Bio Interfaces"
in Biophysics by Denys Biriukov

To write a supervisor's evaluation of Denys Biriukov's thesis and overall doctoral performance is a joyful task. He is smart, hard working, initiative, full of good ideas and a great team member.

Denys very quickly mastered the necessary skills to perform computer simulations and during the years gradually implemented more advanced techniques to cope with the challenging tasks, particularly related to sampling of rare events and overcoming potential energy barriers. He learned to raise and address questions to be answered by computer simulations and linked with results of collaborating experimentalists.

The route to his publications was not as easy as might seem from the final list of publications. His first paper was published 2.5 years after the start of his Ph.D. study, because the anticipated standard task of investigating the adsorption of oxalic acid on rutile surfaces turned non-trivial, recognizing that to model its ions, one needs to apply the Electronic Continuum Correction, which became the central topic of Denys' dissertation. Paving the way to incorporate this approach to simulations of interfaces, the other publications quickly followed, totaling in 6 accepted publications in journals with IF from 3.6 to 4.3 (3 as first author), another one expected to be published soon in J. Mol. Liq. and another one completed on the simulation side but requiring verification of the experimental conditions – not to mention other results to be published, including the study of adsorption of amino acids.

Though (or because) using only computer simulations to obtain data, collaboration with experimentalists is an important part of the research of a computational physicist. Denys' collaboration with experimentalists carrying out surface titration experiments (U of Illinois, Texas Tex U), neutron diffraction (initiated during his month's stay at the Oak Ridge National Laboratory) and second harmonic scattering (EPFL Lausanne) definitely proved that he is able to interact with experimentalists as a valuable team member, enriched both sides and lead to well accepted papers.

I've spent wonderful and stimulating four years with Denys as a student, look forward to a partially continuing collaboration on the project with ORNL – and sincerely wish him a successful postdoctoral position to move on in his career. I believe he has all the prerequisites and potential for a very successful scientific career.

I like the thesis as written. I am convinced, without any reservations, that Denys Biriukov deserves the degree of a doctor in Biophysics.

In České Budějovice, June 9, 2020

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