FACULTY
OF MATHEMATICS
AND PHYSICS
Charles University

Prague, August 21, 2024

Dissertation thesis report

As the PhD advisor of Kryštof Březina, I would like to offer my assessment of his dissertation thesis entitled *"Ab initio and path integral molecular dynamics methodology for hydrogen-bonded systems in the condensed phase"* and of his work as a PhD student under my supervision more generally.

The thesis provides an overview of the main focus of Kryštof's research work with an introduction to the broader area of research, details of the methodology, summary of results, and the student's own perspective on the relevance of the work done. In addition to the thesis itself, the thesis comprises five published articles, with one of them being in the pre-print stage. The student's contributions to each published article are clearly stated. The text of the thesis is written very clearly and in excellent English, with attention to detail and a minimum of typos or similar issues. The chapter on methodology includes more detail than would normally be suitable for a research article, presenting an opportunity for the student to demonstrate his grasp of the methods used in the work. The research chapters offer a guide through the work that is published in the enclosed articles as well as additional detail and discussion of open problems that remain to be addressed in future work. Figures were prepared specifically for the thesis, rather than being re-printed from articles or from previous work, further emphasizing the effort spent on the thesis. Overall, the quality of the work shown in the thesis is excellent.

Kryštof Březina is the first author of four out of the five enclosed articles as well as the main author of the work presented towards the end of the thesis that is currently unpublished. While it is difficult to remain unbiased as the supervisor and the corresponding author of the published work, I would like to say that I am very satisfied not only with the thesis itself but also with the quality of the published research. During his studies, Kryštof was able to learn and become comfortable with a broad range of methods in theoretical and computational physics and chemistry, ranging from electronic structure methods and molecular dynamics methodology to path integrals and machine learning for molecular

Institute of Physics of Charles University
Ke Karlovu 2026/5, 121 16 Praha 2, Czech Republic
fuuk@karlov.mff.cuni.cz
+420 95155 1344, 95155 1461

simulations and a range of computational tools. He was also able to combine this with his understanding of molecular systems and chemistry generally to keep the research relevant to real-world applications. The work is a testament to this growth and demonstrates his ability to contribute to the state of the art in a way that is appreciated by other researchers. Kryštof's approach to research work has been exemplary throughout his time with me. He is always eager to tackle a new problem, strives to understand thoroughly the methods used, and takes initiative in solving research tasks and addressing issues that inevitably arise. As a personal note, I would like to say that I could not be happier with the way the first PhD student fully under my supervision tackled the daunting task of performing the required research and preparing his dissertation thesis.

I have no hesitation in recommending the award of the PhD degree to Kryštof Březina.

RNDr. Ondřej Maršálek, Ph.D.

Institute of Physics of Charles University
Faculty of Mathematics and Physics, Charles University