

Report of a thesis

submitted at the Faculty of Science, University of South Bohemia

supervisor's report

opponent's report

bachelor thesis

master thesis

Author: **Bc. Patrik Musil**

Thesis Title: **Calculation of vibrational SFG spectra from molecular dynamics simulations**

Study program: Physical Measurements and Modelling

Year of submission: 2022 (summer term)

Supervisor: doc. RNDr. Milan Předota, Ph.D.

Workplace: Department of Physics, FSc USB

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Scientific/professional quality:

excellent very good average below average unsatisfactory

Factual errors:

almost none a reasonable number frequent minor errors serious

Results:

original original and adopted non-trivial compilation cited from the literature
 copied

Extent of the work:

large standard sufficient insufficient

Graphic, linguistic, and formal quality:

excellent very good average below average unsatisfactory

Typographic errors:

almost none a reasonable number numerous

Overall quality of the thesis:

excellent very good average below average unsatisfactory

Verbal evaluation:

The topic of the thesis was chosen based on ongoing research, requiring a student capable to modify a code for postprocessing of originally ab initio trajectories to predict sum frequency spectra from classical molecular dynamics simulations. The original code was developed in the group of prof. Marie-Pierre Gaigeot (most recently by Simone Pezzotti) and used with only minimal changes (and all existing limitations) by Ondřej Kroutil.

Patrik Musil perfectly grasped the task, learning quickly FORTRAN language and rewriting the code in a very efficient and nice to read object code. In addition to his programmer's skills, he nearly independently understood the numerous parts of the code based on published theory, requiring just few consultations regarding the calculation of instantaneous surfaces and spectra. In this process, he revealed even unpublished features of the code, namely applied decaying filter function applied to the time-correlation function.

In addition to technical improvements including optimization of the data files, he succeeded in implementing the cross-correlation contributions, dynamic assignment of molecules to interfacial layers, and inclusion of calculations of surface hydroxyls by the same code (as opposed to separate code used by S. Pezzotti). In these aspects, he fulfilled partial goals of a running Czech Science Foundation project.

The big amount of practical work related to modifications and testing of the code (which was from the beginning planned as the key part of this thesis) resulted in a limited time left for thesis writing and applications.

While the thesis describes the work done, it might better explain the motivation for the changes and improvements. Also, the practical examples of application of the code would benefit from analyses of longer simulation trajectories and examples of applications to more systems.

Still, the analyses of the (in)dependence of the results on length of correlation functions, applied smoothing filter, and thermostating provide useful guidance for further analyses.

Based on the above facts, evaluating as excellent the practical part (code development) and having some reservations about the written form of the thesis, I find the thesis of great importance and benefit for the ongoing research.

Patrik Musil successfully proved that he is able to solve problems, identify key points and raise relevant questions, and be a fruitful team member.

Questions to the defense and suggestions for a discussion:

Which further modifications of the code do you find most important to implement as a continuation of your work?

I recommend

~~**I do not recommend**~~

to accept the thesis as a master thesis.

I suggest that the thesis be graded:

excellent very good good failed

Place, date, and signature of the supervisor:

České Budějovice, 18. 5. 2022