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Prague, August 13, 2014

Letter from the PhD. advisor

It is my great pleasure to recommend the PhD. thesis of Frank Uhlig entitled “Structure, dynamics, and reactivity of the hydrated electron” for defense.

Frank started his PhD. work in my group in 2010 after graduating (MSc.) in chemistry at the Leipzig University. He came to Prague as a gifted and skilled quantum chemist with strong inclinations to development of algorithms and a touch of computer wizardry. In our group, I believe we put his skills in good use and, at the same time, allowed him also to develop in the direction of molecular dynamics and acquire more of chemical intuition.

At the early stages of his PhD. work, Frank started working with me and a (at that time) senior student in the group, Ondřej Maršálek, on unraveling the structural, dynamical, and chemical reactivity aspects of electrons solvated in aqueous environments. In due time, Frank took over the project and brought it practically to completion, as exemplified by his most recent paper on the subject recently published in Nature Chemistry. Of course, there are still loose ends (as also mentioned in the thesis) which we are currently trying to tie up and, hopefully, publish in the future. Nevertheless, thanks primarily to Frank and his ab initio molecular dynamics simulations our understanding of hydrated electrons has already been brought up to a new qualitative level. This has been well recognized by the broader scientific community to which Frank communicated his results also in the form of invited lectures and posters at several international conferences (including Gordon research conferences).

Frank's PhD. thesis is built on seven papers, which have been already published in leading international journals and in which he has played a key role. This part is preceded by a thorough introduction to the methodology, summary of the results, and concluding remarks summarizing remaining problems and outlook for future research. The thesis is very well written and should provide a good read for interested scientists, as well as a valuable reference for future students in my group. As such, it should provide an excellent basis for providing Frank the PhD. title.

In conclusion, I hate to see Frank leaving my group, but as a mature young scientific personality he is ready to go and launch the next stage of his scientific career, a postdoctoral stay.

Sincerely

A handwritten signature in blue ink, appearing to read 'Pavel Jungwirth', with a stylized flourish at the end.

Prof. Pavel Jungwirth