

Prague, August 27th 2013

Advisor's report on doctoral thesis of RNDr. Lukáš Grajciar

Lukáš Grajciar has been in my group for more than 7 years. During this time I've been his advisor for Bachelor thesis, for Diploma thesis, and since 2009 I am his advisor for PhD thesis. Lukáš's dissertation entitled "Quantum-chemical study of adsorption in microporous materials" is based on the results reported previously by Lukas in one book chapter and in 7 scientific papers published in excellent international journals (J. Phys. Chem. Letters, J. Phys. Chem. C, Chem. Phys. Chem., Chem. Sus. Chem., Phys. Chem. Chem. Phys.). These results are summarized on about 50 pages together with very well written overview of dispersion-corrected density functional theory based methods. Lukáš has participated in the model and method development and he applied state-of-art methods to the description of adsorption in microporous materials. Lukáš has substantially contributed in solving parts of 7th FP project MACADEMIA where he has achieved highly accurate description of metal organic frameworks and their interactions with adsorbates. His contribution in the field is well recognized (his work has been cited 117 times without self-citation) and his work on CuBTC metal organic framework now sets the benchmark for other computational investigations.

Among the PhD students I have been advising so far (total of seven PhD students) Lukáš Grajciar was the best student with great academic potential. He has always had excellent study record and he has always taken more courses and exams than required. To improve his background in math and physics Lukáš has taken bachelor courses in Faculty of Math and Physics in parallel with his doctoral studies in Faculty of Science. Regardless of his large studying load Lukáš has worked hard also on his scientific tasks and he has been able to finish many scientific projects as it is documented by a relatively large number of publications co-authored by him (discussed below). Lukáš has shown a great studying capability, he has developed a very high technical skills and he has, according to my opinion, a great academic potential.

So far Lukáš has published 12 papers in very good international journals, and he is the first author on 5 of them. In all the papers where he was the first author he was responsible for computational part of the investigation and he had a major contribution in writing the paper. His independence in solving scientific tasks and in writing reports/papers has improved over the time and now he can be considered independent young researcher. Lukáš has also taken a major part in writing one book chapter (submitted). In addition to 12 papers already published, there is one manuscript co-authored by Lukáš submitted and he is currently involved in finishing two more publications. Overall, during his study Lukáš has been co-authoring 15 papers and one book chapter.

During his PhD study Lukáš has proved his ability to participate in the method development as well as in their application on particular problems. Aside the scientific quality of the

applicant I would like to mention his reliability and responsibility for the work he has done. Lukáš has always met the project deadlines.

According to my opinion RNDr. Grajciar is clearly shaping up his research profile; his expertise is on the borderline between method development and applications with the emphasis on highly accurate calculations of material properties. His dissertation meets the highest standard and I am pleased to recommend his work for defense.

Doc. Petr Nachtigall