

March 15, 2021

Opinion of the PhD thesis supervisor

Mgr. Andrej Antalík worked in my group already as a master student and defended his master thesis entitled “Density matrix renormalization group calculations and entanglement optimization in quantum chemistry” in 2015 and subsequently he continued with a PhD study on the topic of “Coupled clusters tailored by matrix product state wave functions”.

During his doctoral study, Andrej Antalík implemented the DMRG-tailored CC method within the computationally efficient domain-based local pair natural orbital formalism, at the level of single, double and perturbative triple excitations. He successfully applied the method to study of several strongly correlated molecular systems, where the importance of a balanced description of static and dynamic correlation has been demonstrated.

The submitted thesis consists of a well written introduction to the topic and description of the theoretical methods involved as well as presentation of some of the numerical results, with reprints of six relevant publications in peer reviewed journals attached (on three of them he is the first author). In total, Andrej Antalík has coauthored 11 publications, which have been 119 times cited in total (101 self-free), yielding h-index 6.

In my opinion, Andrej Antalík is a very bright student, working hard and with a deep interest in the topic, bringing his own invention and initiative. I am firmly convinced that his achievements so far proved beyond doubt that he is a talented young researcher and I thus strongly recommend his thesis to be accepted for defense and after a successful disputation to award him the PhD title.

Doc. Mgr. Jiří Pittner, Dr. rer. nat., DSc.