19.3.2024

To: Prof. Zdeněk Doležal, Faculty of Mathematics and Physics, Charles University, Czech Republic

Evaluation of the Habilitation Thesis of Dr. Zdenek Futera

Title of the thesis "Computational Approaches to Electron Transfer Processes: From Ionic Solutions to Nanobioelectronic Devices"

The Habilitation Thesis of Dr. Zdenek Futera focuses on molecular level modelling of the electron transfer (ET) process. Electron transfer is a complex quantum mechanical process and its modelling is far from easy. (Rudy Marcus, Nobel Prize in Chemistry, for the theory of electron transfer reactions in chemical systems, 1992). ET is important in many fields of science, including chemistry and biochemistry. The current computers and software make it possible to perform realistic simulations of the ET process in various chemical environments. Dr. Futera has a very good focus area for modern research.

The thesis of Dr. Futera shows that he has an excellent knowledge of molecular modelling of ET. The summary of the thesis is a coherent and up-to-date review of various aspects of electron transfer both from the theory and the computational sides. The summary also address methods to model the molecules movement, like MD, AIMD and QM/MM. He has also very good knowledge of computational tools to solve the ET problems and he has participated in the development of these tools.

Dr. Futera has listed 14 high-quality research papers to demonstrate his recent research. Many of these papers address challenging research problems. He has been working with Prof. Blumberger who is one of the leading researchers in ET modelling and they have several joint papers. Dr. Futera has also worked with prof. English. In these collaboration publications, Futera has clearly listed his contribution and in all these publications he has had important and original contributions. I also searched Dr. Futera's recent scientific publications (from Web of Science) and his publication activity is very good, several good quality publications per year.

The summary and listed papers show that Dr. Futera has studied ET in an impressive number of systems, including atom-atom (in water), surface-molecules and complex biochemical molecule-molecule ET. Overall, he has a very solid background in his research. In addition to the challenging simulation projects he has participated in the development of some of the computational tools which is an important aspect of leading-edge research.

Most of the selected publications have been done in collaboration with senior scientists but he has recently established his own research group and he has also publications coming from his group. This is a good indicator of independent research.

To summarize Dr. Futera's recent research has been of very high quality. He has done several very interesting and challenging simulations in an important research field. He clearly has

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increased the scientific knowledge and has become a world-class expert in his own subfield of science. He has shown that he can conduct independent research.

In teaching, Dr Futera has given several courses. These include courses related to his expertise, such as Density Functional Theory and Electron Transfer Processes but also more general courses Physics I and Programming. This is a balanced set of courses and he has taught these courses several times. I do not have information on Student Feedback for these courses or a more general Teaching Portfolio. I see that his teaching activities are sufficiently broad.

The reviewer was also asked to comment on the output of the plagiarism check. The overall thesis match is high since the thesis contains several published articles. The more detailed matches are mostly due to Futera's own articles stored in various repositories. There are few very low level matches on other research articles related to ET. I do not see any sign of plagiarism in this thesis.

I will strongly recommend progressing Dr. Futera's habilitation procedure. His Habilitation thesis is of very high quality and it is based on several high quality original research publications. He can lead an independent research group and his teaching is of sufficient level. If that matters, he would be eligible for a (junior) professor position at Aalto University and other similar level good research universities.

Espoo, Finland 19.3.2024

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