**Opponent's review of the Zdenek Futera habilitatio thesis**

**Computational Approaches to Electron Transfer Processes:**

**From Ionic Solutions to Nanobioelectronic Devices**

In habilitation thesis Zdenek Futera shows the diverse mechanisms by which charge can be transferred in various materials, with a specific emphasis on electronic transfer in molecular systems, particularly those facilitated by biomolecules. Author explains how and why various mechanisms play role in different contexts and materials, highlighting the complexity and versatility of charge transfer processes.

Zdenek Futera has been involved in significant work concerning the methodology development for studying biomolecular charge transfer. This includes various techniques such as the design of computational methods, implementation of algorithms, and refinement of force fields tailored for investigating electron transfer processes within biomolecular systems.

Additionally, Futera has applied these methodologies to study electron transfer in a diverse range of systems, both biologically relevant and beyond. By presenting selected applications, with part focusing on biologically relevant systems and the other part on different systems. The work highlights the versatility and effectiveness of the developed methodologies in elucidating fundamental processes governing electron transfer dynamics.

Moreover, the relevance and significance of Futera research are supported by the publication of relevant articles in peer-reviewed journals, indicating that their findings have undergone validation within the scientific community. This demonstrates Futera's contributions to advancing our understanding of biomolecular charge transfer phenomena and their broader implications in various scientific domains. Finally, the main applications focused on electron transfer in various systems are introduced as successful study cases.

The quality of Zdenek Futera's work is further evidenced by the fact that he is a co-author of a number of original works published in prestigious scientific journals. Besides these research activities, the author participate in education of students at Faculty of Science at University of South Bohemia. There, at Department of Physics, he established two new courses: ”Density Functional Theory (DFT) and Its Applications” and ”Charge Transfer Processes and Their Simulations”. Based on the check of the originality of the habilitation thesis carried out by the Turnitin system, it is clear that there is certain but acceptable overlap with the existing literature written by the author.

As the work meets the standard requirements for habilitation thesis I recommend the work for further progress in the habilitation procedure.

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