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Bc. Nicole Bradfordová  
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Dear Ms. Bradfordová,

I am delighted to provide my assessment of the habilitation thesis of Dr. Lukáš Grajciar (hereafter referred to as *author*) entitled *Towards reliable simulations of nanoporous materials under operando conditions*. The self-report format of the thesis supported by an extensive list of references, which is divided into six main chapters, is an original testimony to the author's in-depth knowledge of the subject matter.

The author's involvement in the development of new methods and their application to porous nanomaterials is an outstanding achievement. The fourteen peer-reviewed articles that resulted from this research, including publications in prestigious journals such as *Nature Communications* and *Chemical Society Reviews*, demonstrate the quality and significance of the author's work. These publications also attest to the author's exceptional research skills and the impact of his contributions on the field, including zeolites and metal-organic frameworks. Additionally, I would like to highlight the author's contribution to the development and use of machine learning approaches in his research.

The first chapter of the thesis introduces the subject matter and outlines the research objectives. The second chapter describes the methodology used in the research, including the author's role in the methods development. The third chapter highlights the author's application results in nanoporous materials, and I value the specification of author's contribution to the specific topic, including a list of related articles, the importance of the research in the broader context, and the outlook of the methodological development or application finding. The fourth chapter presents the author's conclusions and recommendations for future research, specifically in the context of machine-learning methods. The fifth chapter contains a bibliography, which is a helpful resource for readers. Finally, the sixth chapter provides a list of papers the thesis is built upon.

Overall, the habilitation thesis is a comprehensive and well-organized examination of computational studies of porous nanomaterials. The author's research and publications demonstrate his expertise and competence in the field, and his contributions to the method development and their applications are of significant scientific and practical importance. The thesis also highlights the author's exceptional ability to communicate complex concepts in a clear and concise manner.

In summary, Dr. Lukáš Grajciar's habilitation thesis is a remarkable accomplishment, and I fully endorse a positive conclusion of the habilitation process. The author's research and publications have significantly advanced the field of computational studies of porous materials, and his work will undoubtedly continue to have a profound impact on the scientific community for years to come. I wish Dr. Grajciar a brilliant scientific future.

Yours Sincerely,

Doc. Mgr. Piotr Błoński, Ph.D.