Department of Physical and Macromolecular Chemistry
invites you to a seminar and a habilitation lecture

Towards reliable simulations of zeolites under operating conditions

Lecture hall CH3, Faculty of Science, Hlavova 8, Praha 2

on October 18th, 2023 at 14:00

speaker: RNDr. Lukáš Grajciar, Ph.D.

Zeolites, the crystalline (alumino)silicates, are materials produced at the Megaton scale with commercial applications ranging from detergents through thermal energy storage to catalysis. Even though zeolites have been studied for decades, understanding of their dynamical behaviour at operating conditions at the molecular level, including their (trans)formation and decomposition mechanisms is still mostly lacking.

In this habilitation lecture, the advanced simulation methodologies (e.g., biased ab initio molecular dynamics or machine learning accelerated simulations) capable of bridging this gap will be briefly outlined. In the last part, the potential of these methodologies will be highlighted in studies focused on the reactive zeolite-water interactions, which are pivotal to optimize synthesis and production processes, increase the zeolites' durability and facilitate the design of new zeolites with superior property profile.

Organizers: Prof. Tomáš Obšil, Dr. Ondřej Sedláček

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