Static and dynamic fluid properties in mesoporous confinement

Marc Högler[1], Hamzeh Kraus[1], Niels Hansen[1]

[1]Institute of Thermodynamics and Thermal Process Engineering, Pfaffenwaldring 9, D-70569 Stuttgart, Germany

E-Mail presenting author: marc.hoegler@itt.uni-stuttgart.de

Mesoporous materials play an important role as catalyst support. Due to the confinement effect, they can for example influence the selectivity of a chemical reaction. A fundamental understanding of mesoporous materials allows design adjustments to improve the performance of the catalytic reaction. Molecular simulation techniques can be used in conjunction with experimental data to study physical processes inside mesopores in more detail. We are developing an open-source software tool referred to as PoreMS to create silica pores for moleculear dynamics (MD) simulations [1]. The generated structures can then be used to examine a wide variety of systems. For this purpose, we developed another Python package called PoreSim, which provides a complete setup for the MD simulation program GROMACS to run the system. The third package PoreAna enables the analysis of the simulated trajectory and provides density and diffusion profiles. Using the workflow, the influence of complex silica structures with different surface occupancy or diameter on diffusion under confinement can be considered. Various systems have also been inverted, such as supported ionic liquid phase systems in mesoporous silica confinement.

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[2] T. Kobayashi, H. Kraus, N. Hansen, M. Fyta, *ChemCatChem* 2021, *13*, 739-746