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Confinement effects induced by pore surface roughness on Knudsen diffusion in amorphous mesoporous materials: An experimental study

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The roughness of the internal surface of porous media is a form of static geometrical heterogeneity that influences the molecular trajectories of gas molecules moving through them. The perturbations along the pore walls reduce the accessibility of the surface area and cause temporary trapping effects. The surface roughness of the pore walls is responsible for non-negligible confinement effects in amorphous mesoporous materials (2-50 nm pore diameter), such as those used for catalysis and separation processes [1], where Knudsen diffusion is often the limiting transport mechanism in mesopores. In Knudsen diffusion, the interactions between the gas molecules and the pore walls are significant.
The investigation of the effect of surface roughness of porous media on Knudsen diffusion was conducted by Coppens and co-workers [2] and Zschiegner et al. [3] using analytical calculations and computer simulations. In their work, single pore models of fractally rough pores are used to model the pore geometry. A significant decrease in the Knudsen diffusivity has been predicted with increased surface roughness. For the experimental validation of these results, an Ultra-High Vacuum Diffusion Setup was built as a scale-up of the pore [4] . Such a setup uses ultra-high vacuum conditions with the same Knudsen number (ratio of mean free path to local channel diameter) as in the mesopore and a 3D-printed channel. The channel contains random Koch fractal segments to create the internal channel surface, which simulates the fractal surface roughness of the mesopore walls.

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Primary author: MOURKOU, Maria (University College London (UCL))

Co-authors: YU, Haiyue (University College London (UCL)); COPPENS, Marc-Olivier (University College London (UCL))

Presenter: MOURKOU, Maria (University College London (UCL))

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