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Concentration-dependent self-diffusion of adsorbates in mesoporous materials

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Abstract

The pulsed-field gradient NMR method has been applied to study self-diffusion of liquids in mesoporous materials with different pore sizes and morphologies as a function of pore loading. It is found that the effective diffusivities of adsorbate molecules in mesopores at partial loadings are related to two mechanisms, the Knudsen diffusion through the gaseous phase in the pore space and the diffusion within the layer of molecules adsorbed on the pore walls. The relative contributions of these modes, which are determined by the details of the interphase equilibrium, change with variation of the pore loading, leading to a complex behavior of the effective self-diffusion coefficient. The impact of the pore size and the adsorbate-surface interaction on self-diffusion is elucidated. Possible reasons for an experimentally obtained hysteresis in the diffusivities measured on adsorption and desorption in mesopores are discussed.

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Keywords

Adsorption isotherm, Concentration, Hysteresis, Porous materials, Self-diffusion