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Argon Adsorption in Three-Dimensional Ordered Mesoporous (3DOm) Carbons: Monte Carlo Molecular Simulation Study MAX A. MAXIMOV, GENNADY GOR, New Jersey Inst of Tech — Templated nanoporous materials show excellent performance in many applications due to well-defined pore sizes and morphologies. 3DOm carbons are prepared using silica-nanospheres as a template, thus they have spherical pores interconnected by circular windows. Recent experiments show that 3DOm carbons work efficiently as a medium for storing methane in the pores in the form of hydrates. However, the basics of this process are not clear, and in particular it is not known how the pore morphology affect formation of hydrates. Moreover, even behavior of simpler fluids (nitrogen and argon) in 3DOm carbons, is not well understood. Adsorption of these two fluids is routinely used for characterization of nanoporous materials, and correct physical interpretation is required to extract the pore-size distribution from the experimental adsorption data. Here we present the Monte Carlo molecular simulation study of argon adsorption in 3DOm carbons. To represent 3DOm structure, we use two models: an ideal spherical pore, and a system of spherical pores, connected with the openings. Our simulations show that the openings between the pores are necessary for the analysis of experimental adsorption data. Our results also serve as a starting point for modeling hydrate formation in 3DOm carbons.

Max Maximov
New Jersey Inst of Tech

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