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Kinetics of Gas Adsorption in Nanopores: A Computer Simulation Study CHRISTOPHER E. PUEBLO, Southern Illinois University Carbondale, M. MERCEDES CALBI, University of Denver — Motivated by a variety of experimental results concerning gas adsorption in open-ended carbon nanotubes, we present a series of results for the kinetics of adsorption of a gas inside a nanopore. The study is based on a Kinetic Monte Carlo simulation in combination with a lattice model of adsorption. This allows us to monitor the change in coverage with time and extract corresponding adsorption rates or equilibration times. Adsorption in nanopores presents several distinctive features when compared to open surfaces. The adsorption process is mainly controlled by the energy states close to the ends of the pore; we analyze the consequences of this effect on the equilibration times of the system and also on temperature programmed desorption spectra.

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