

Abstract Submitted
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Kinetic Monte Carlo study of gas transport through a nanopore¹

JOSHUA VANN, M. MERCEDES CALBI, University of Denver — We investigate the gas transport through a narrow pore by implementing a Kinetic Monte Carlo simulation on a single line of sites. Adsorption processes are restricted to the end sites that are in contact with gas reservoirs at different pressures. Particles gain access to the interior of the pore by hopping between the lattice sites. We follow the total uptake change with time as the system evolves to equilibrium, and we also examine the distribution of the particles along the pore at different times in the evolution. We analyze the overall dynamic behavior of the adsorbed phase in terms of the occurrence of the elementary processes that drive the system to equilibrium.

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