Carbon dioxide transport in carbon nanopores

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Abstract

In the present study atomistic simulations are employed for investigating the CO_2 transport properties through pores that are of slit, cylindrical and scroll configuration. We aim to investigate any possible differences in the adsorption process among the three different geometries focusing on the adsorption type that occurs along with pore filling and pore emptying mechanisms. Carbon-slit pores are of widths between 0.8 and 2.0 nm. The simulated Single-Walled Carbon Nanotubes (SWNTs) are of 1.08 and 2.17 nm ((8,8) and (16,16) respectively) while for the Carbon Nanoscrolls (CNSs) the inner diameter corresponds to a (6,6) SWNT with an intralayer distance of 0.4 to 1.0*nm*.