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Grand Canonical Monte Carlo simulations of the uptake of gases inside Single Wall Carbon Nanotubes BRYAN RAMSON, SILVINA GATICA, Howard University — Gases adsorbed in the interior of open-end carbon nanotubes have different characteristics depending on the size of the molecules, diameter of the nanotubes interaction potentials, temperature and chemical potential. For example, at low temperature and low coverage H_2 is deposited on a shell against the internal carbon wall, and populates the center of the tube only at a higher chemical potential. The porpuse of the present work is to estimate the conditions necessary for a signigicant uptake and for capillary condensation of different species in different-size of tubes. For example, at a temperature of 120 K, the uptake of Ar starts at a pressure P $=10^{-4}$ atm, while for Helium a pressure of 1 atm is needed to start the adsorption. The conditions for adsorption and configurations of the adsorbate are dramatically different for a different set of parameters. In this work we calculated the uptake for Ar, Kr, Ne, CH_4, Xe, He and H_2 in a broad range of pressures, temperatures and diameter of the nanotubes. We also studied the phases, configurations and energies.

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